Access DB# 123804

4 SEARCH REQUEST FORM

Scientific and Technical Information Center

5/18/99

Requester's Full Name: HARDEE Examiner # : _____ Date: 6/04

Art Unit: 1751 Phone Number 30 21318 Serial Number: 09/980,641

Mail Box and Bldg/Room Location: 9A41 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

Whatever you can find.
Thanks

33 ✓
3+ more
5+

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STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher: EA	NA Sequence (#):	STN: $296.55
Searcher Phone #:	AA Sequence (#):	Dialog:
Searcher Location:	Structure (#):	Questel/Orbit:
Date Searcher Picked Up:	Bibliographic: ✓	Dr Link:
Date Completed: 6-4-04	Litigation:	Lexis/Nexis:
Searcher Prep & Review Time: 5	Fulltext:	Sequence Systems:
~~Clerical Prep Time:~~	Patent Family:	WWW/Internet:
Online Time: 65	Other:	Other (specify):

PTO-1590 (8-01)

09/980641

JC10 Rec'd PCT/PTO 15 NOV 2001

PATENT
Attorney Docket No. INE 109

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of:
Robin Riyadh GIBSON and
Greg Lyndon SUMMERS

International Application No.:
PCT/GB00/01861

International Application Filing Date:
May 15, 2000

Priority Date: May 18, 1999

For: PRODUCTION OF 1,1,1,2,3,3,3-HEPTAFLUOROPROPANE

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Date of Deposit November 15, 2001

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NAME Yue Yo Ruan
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SIGNATURE Yue Yo Ruan

Commissioner for Patents
Washington, D.C. 20231

PRELIMINARY AMENDMENT

Dear Sir/Madam:

Please enter this Preliminary Amendment prior to calculating the filing fee.

IN THE CLAIMS:

Please amend Claims 1, 5 and 8 as follows:

1 (Amended). A process for the production of 1,1,1,2,3,3,3-heptafluoropropane (HFC 227ea) by the reaction of hexafluoropropene (HFP) with hydrogen fluoride characterised by the Steps of

A. charging the reaction mixture from the reaction of HFP with hydrogen fluoride to a liquid-phase separator and

allowing an organic phase and a hydrogen fluoride-rich phase to separate under gravity;

B. recycling the hydrogen fluoride-rich phase separated in Step A to the reactor in which the reaction is carried out:

C. charging the organic-rich phase separated in Step A to a distillation column;

D. recovering the HFC 227ea and an hydrogen fluoride-rich mixture separately from the distillation column in Step (C); and

E. recycling the hydrogen fluoride-rich mixture recovered from Step D to the reactor.

5 (Amended). A process according to Claim 1 in which HFP in addition to that present in the reaction mixture from the reaction of HFP with hydrogen fluoride is introduced into the process.

8 (Amended). A process as claimed in Claim 1 wherein the mixture to be separated in the liquid-phase separator in Step (A) comprises a mole ratio of HF:HFC 227ea of between 3:7 and 6:4.

REMARKS

This is a Preliminary Amendment to the above-identified patent application. In Claim 1, the second occurrence of "hexafluoropropane" has been deleted and replaced with --

Claims

1. A process for the production of HFC 227ea by the reaction of HFP with hydrogen fluoride characterised by the Steps of
   A. charging the reaction mixture from the reaction of HFP with hydrogen fluoride to a liquid-phase separator and allowing an organic phase and a hydrogen fluoride-rich phase to separate under gravity ;
   B. recycling the hydrogen fluoride-rich phase separated in Step A to the reactor in which the reaction is carried out:
   C. charging the organic-rich phase separated in Step A to a distillation column;
   D. recovering the HFC 227ea and an hydrogen fluoride-rich mixture separately from the distillation column in Step (C); and
   E. recycling the hydrogen fluoride-rich mixture recovered from Step D to the reactor.
2. A process as claimed in Claim 1 wherein the reaction mixture charged to the liquid-phase separator in Step (A) comprises an HFC 227ea/HF azeotrope, or azeotrope-like mixture.
3. A process as claimed in Claim 1 wherein in Step A the organic phase and the hydrogen fluoride-rich phase are allowed to separate under gravity at below ambient temperature.
4. A process as claimed in Claim 1 wherein in Step A the organic phase and the hydrogen fluoride-rich phase are allowed to separate under gravity at supra-atmospheric pressure.
5. A process as claimed in Claim 1 further characterised in that the HFP is charged to the liquid-phase separator.
6. A process as claimed in Claim 1 further characterised in that the HFP is charged to the reactor.
7. A process as claimed in any one of the preceding claims wherein the mixture to be separated in the liquid-phase separator in Step (A) comprises a mole ratio of HF:HFC 227ca of between 3:7 and 6:4.

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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                  E HEXAFLUOROPROPENE/CN
L2                1 SEA HEXAFLUOROPROPENE/CN
                  E HYDROGEN FLUORIDE/CN
L3                1 SEA "HYDROGEN FLUORIDE"/CN

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L9             1085 SEA L2 (L) RACT/RL
L10            6955 SEA L3 (L) RACT/RL
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L18       108345 SEA HF
L19           39 SEA L13 AND (L15 OR HEXAFLUOROPROPENE# OR HFP) AND (L17
                 OR L18 OR HYDROGEN#(W)(FLUORIDE# OR MONOFLUORIDE#) OR
                 HYDROFLUORIC#(A)ACID#)
L20       367107 SEA DISTILL? OR DIST# OR DISTN# OR CODISTILL? OR CODIST#
                 OR CODISTN# OR AZEOTROP? OR COAZEOTROP?
L21           12 SEA L19 AND L20
L22           24 SEA L11 OR L21
L23           15 SEA (L7 OR L19) NOT L22


=> file hca
FILE 'HCA' ENTERED AT 18:00:09 ON 04 JUN 2004
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=> d l22 1-24 cbib abs hitstr hitind

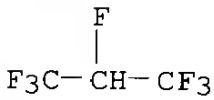
L22  ANSWER 1 OF 24  HCA  COPYRIGHT 2004 ACS on STN
140:237530  Processes and catalysts for the preparation of
     2-chloro-1,1,1,2,3,3,3-heptafluoropropane, hexafluoropropene and
     1,1,1,2,3,3,3-heptafluoropropane.  Nappa, Mario J.; Rao, Velliyur
     Nott Mallikarjuna; Rosenfeld, H. David; Subramoney, Shekhar;
     Subramanian, Munirpallam A.; Sievert, Allen C. (E.I. du Pont de
     Nemours and Company, USA).  PCT Int. Appl. WO 2004018397 A1
     20040304, 29 pp.  DESIGNATED STATES: W:  AE, AG, AL, AM, AT, AU, AZ,
     BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ,
     EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE,
     KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
     MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
     SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM,
     ZW, AM, AZ, BY, KG, KZ, MD, RU; RW: AT, BE, BF, BJ, CF, CG, CH, CI,
     CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE,
     NL, PT, SE, SN, TD, TG, TR.  (English).  CODEN: PIXXD2.
     APPLICATION: WO 2003-US26331 20030821.  PRIORITY: US 2002-PV405222
     20020822.
AB   A process for the prepn. of 2-chloro-1,1,1,3,3,3-heptafluoropropane
     is described which involves: (a) contacting a mixt. comprising
     hydrogen fluoride, chlorine, and at least one starting material
     selected from halopropenes CX3CCl:CX2 (X = F, Cl; Y = H, Cl, F;
     provided that the no. of X and Y which are F totals ≤6) and
     halopropanes CX3CClYCX3, where each with a chlorofluorination
     catalyst in a reaction zone to produce a product mixt. comprising
```

CF3CClFCF3, HCl, HF, and underfluorinated halogenated hydrocarbon intermediates. The chlorofluorination catalyst comprises at least one chromium-contg. component selected from (i) a cryst. alpha-chromium oxide where at least 0.05 atom% of the chromium atoms in the alpha-chromium oxide lattice are replaced by nickel, trivalent cobalt or both nickel and trivalent cobalt, provided that no more than 2 atom% of the chromium atoms in the alpha-chromium oxide lattice are replaced by nickel and that the total amt. of chromium atoms in the alpha-chromium oxide lattice that are replaced by nickel and trivalent cobalt is no more than 6 atom% , and (ii) a fluorinated cryst. oxide of (i). Also described is a process for the manuf. of a mixt. of HFC-227ea and hexafluoropropene by reacting a starting mixt. comprising CFC-217ba and hydrogen in the vapor phase at an elevated temp., optionally in the presence of a hydrogenation catalyst.

IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes and catalysts for the prepn. of 2-chloro-1,1,1,2,3,3,3-heptafluoropropane and hexafluoropropene and 1,1,1,2,3,3,3-heptafluoropropane)

RN 431-89-0 HCA

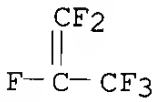
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4P**, Hexafluoropropene
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); **RACT (Reactant or reagent)**
(processes and catalysts for the prepn. of 2-chloro-1,1,1,2,3,3,3-heptafluoropropane and hexafluoropropene and 1,1,1,2,3,3,3-heptafluoropropane)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(processes and catalysts for the prepn. of 2-chloro-1,1,1,2,3,3,3-heptafluoropropane and hexafluoropropene and 1,1,1,2,3,3,3-heptafluoropropane)

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

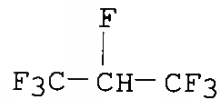
HF

IC ICM C07C017-20
ICS C07C017-21; C07C017-23; C07C019-10; C07C021-18; B01J023-86
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67
IT 422-86-6P 431-86-7P **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane 661-97-2P, 1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane 1652-80-8P
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes and catalysts for the prepn. of 2-chloro-1,1,1,2,3,3,3-heptafluoropropane and hexafluoropropene and 1,1,1,2,3,3,3-heptafluoropropane)
IT 76-18-6P, 2-Chloro-1,1,1,2,3,3,3-heptafluoropropane **116-15-4P**, Hexafluoropropene
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); **RACT (Reactant or reagent)**
(processes and catalysts for the prepn. of 2-chloro-1,1,1,2,3,3,3-heptafluoropropane and hexafluoropropene and 1,1,1,2,3,3,3-heptafluoropropane)
IT 431-52-7 1333-74-0, Hydrogen, reactions **7664-39-3**, Hydrogen fluoride, reactions 7782-50-5, Chlorine, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(processes and catalysts for the prepn. of 2-chloro-1,1,1,2,3,3,3-heptafluoropropane and hexafluoropropene and 1,1,1,2,3,3,3-heptafluoropropane)

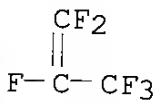
L22 ANSWER 2 OF 24 HCA COPYRIGHT 2004 ACS on STN
139:199086 Processes for the purification and production of fluoroalkanes. Brandstater, Stephan M.; Cohn, Mitchel; Hedrick, Victoria E.; Iikubo, Yuichi (PCBU Services, Inc., USA). PCT Int. Appl. WO 2003068716 A1 20030821, 28 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-US3962 20030211. PRIORITY: US 2002-75560 20020214.
AB Processes that utilize an olefinic compd., in particular, **hexafluoropropene** (**HFP**) or chlorotrifluoroethene

(CFC-1113) as extg. agents in the purifn. of pentafluoroethane (HFC-125) are described. These processes can utilize recovered **HFP** as a precursor for the prodn. of heptafluoropropane (**HFC-227**) or other derivs.

IT **431-89-0P, 2-Hydroperfluoropropane**
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes for the purifn. and prodn. of fluoroalkane)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4, Hexafluoropropene**
RL: NUU (Other use, unclassified); RCT (Reactant); **RACT (Reactant or reagent)**; USES (Uses)
(processes for the purifn. and prodn. of fluoroalkanes)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride**, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(processes for the purifn. and prodn. of fluoroalkanes using)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM C07C017-386
ICS C07C019-08; C07C017-383; C07C021-18; C07C017-087; C07C017-21; C08C019-12
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48
ST pentafluoroethane purifn extractive **distn**; heptafluoropropane prepn purifn; **azeotropic distn** fluoroalkane purifn
IT **Distillation**
(**azeotropic**; processes for the purifn. and prodn. of fluoroalkanes using)

IT **Distillation**
(extractive; processes for the purifn. and prodn. of fluoroalkanes using)

IT **431-89-0P, 2-Hydroperfluoropropane**
2252-84-8P, Propane, 1,1,1,2,2,3,3-heptafluoro- 33660-75-2P, Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes for the purifn. and prodn. of fluoroalkane)

IT **116-15-4, Hexafluoropropene**
RL: NUU (Other use, unclassified); RCT (Reactant); **RACT (Reactant or reagent)**; USES (Uses)
(processes for the purifn. and prodn. of fluoroalkanes)

IT **7664-39-3, Hydrogen fluoride**, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(processes for the purifn. and prodn. of fluoroalkanes using)

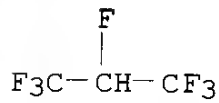
L22 ANSWER 3 OF 24 HCA COPYRIGHT 2004 ACS on STN
138:370659 Regioselective vapor-phase production of **1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**. Miller, Ralph Newton; Nappa, Mario J.; Toton, Donald J. (E. I. Du Pont de Nemours & Co., USA). PCT Int. Appl. WO 2003037832 A2 20030508, 11 pp. DESIGNATED STATES: W: CN, DE, ES, GB; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-US35061 20021031. PRIORITY: US 2001-PV339923 20011031.

AB A process for producing **1,1,1,2,3,3,3-heptafluoropropane** (I) comprises: (a) reacting **hexafluoropropylene** and **HF** in the vapor phase in a reaction zone in the presence of I and a fluorination catalyst (e.g., chromium oxide prepd. by the pyrolysis of ammonium dichromate); (b) feeding the reaction mixt. into a **distn.** column to form a **distn.** column overhead stream of **HF** and I and a **distn.** column bottom stream of I which is substantially free of **HF**; (c) recycling at least a portion of the **distn.** column overhead stream back to the reaction zone; and (d) recovering the **HF**-free I from the **distn.** column bottom stream. This process takes advantage of an **azeotropic** compn. of **HF** and I in order to produce I essentially free of **HF** and to recycle the unreacted **HF** back to the reactor. The recycle of this **azeotropic** compn. also enables the use of I as a diluent to aid in control of reactor temp. for this highly exothermic hydrofluorination reaction (no data).

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**

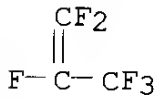
RL: EPR (Engineering process); IMF (Industrial manufacture); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process); USES (Uses)
(regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4, Hexafluoropropylene**
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride**, reactions
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); RGT (Reagent); PROC (Process); **RACT (Reactant or reagent)**
(regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM C07C
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 23, 48
ST heptafluoropropane manuf regioselective hydrofluorination **hexafluoropropylene**
IT **Distillation**
(**azeotropic**; in a regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT **Distillation** columns
(in a regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT Thermal decomposition
(of ammonium dichromate into chromium oxide which is a regioselective hydrofluorination catalyst used in the vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT Process control
(of highly exothermic hydrofluorination by using **1,1,1,2,3,3,3-heptafluoropropane** as a diluent in the regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT Regiochemistry
(regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT Hydrofluorination catalysts
(regioselective; chromium oxide prepd. by the pyrolysis of ammonium dichromate in a regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT Hydrofluorination
(regioselective; regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT 7789-09-5, Ammonium dichromate
RL: EPR (Engineering process); PEP (Physical, engineering or

chemical process); RGT (Reagent); PROC (Process); RACT (Reactant or reagent)
(pyrolysis of ammonium dichromate into chromium oxide which is a regioselective hydrofluorination catalyst used in the vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT 11118-57-3P, Chromium oxide
RL: CAT (Catalyst use); EPR (Engineering process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PREP (Preparation); PROC (Process); USES (Uses)
(regioselective hydrofluorination catalyst in a vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
RL: EPR (Engineering process); IMF (Industrial manufacture); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process); USES (Uses)
(regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT **116-15-4, Hexafluoropropylene**
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT **7664-39-3, Hydrogen fluoride,** reactions
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); RGT (Reagent); PROC (Process); **RACT (Reactant or reagent)**
(regioselective vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

L22 ANSWER 4 OF 24 HCA COPYRIGHT 2004 ACS on STN
138:355466 Vapor-phase production of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**. Miller, Ralph Newton; Nappa,

Mario J.; Toton, Donald J. (USA). U.S. Pat. Appl. Publ. US 2003088132 A1 20030508, 6 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-285193 20021031. PRIORITY: US 2001-PV339923 20011031.

AB A vapor-phase, regioselective process for the prodn. of **1,1,2,3,3,3-heptafluoropropane** (I) from **hydrogen fluoride** and **hexafluoropropylene** in the presence of a chromium oxide catalyst is described which takes advantage of the **azeotropic** compn. of **HF** and I so as to produce I essentially free of **HF** and to recycle the unreacted **HF** back to the reactor. The recycle of the **azeotropic** compn. also enables the use of I as a diluent to aid in control of the reactor temp. during this highly exothermic hydrofluorination reaction; a process flow diagram is presented.

IT **7664-39-3, Hydrogen fluoride,** reactions
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); RGT (Reagent); PROC (Process); **RACT (Reactant or reagent)**
(vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

RN 7664-39-3 HCA

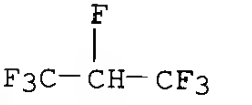
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PREP (Preparation)
(vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

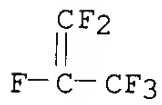
RN 431-89-0 HCA

CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4, Hexafluoropropylene**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); PROC (Process); **RACT (Reactant or**

reagent)
(vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C017-08
ICS C07C019-08
NCL 570164000
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67
ST heptafluoropropane manuf regioselective hydrofluorination **hexafluoropropylene; azeotropic distn**
heptafluoropropane manuf regioselective hydrofluorination **hexafluoropropylene**
IT **Distillation**
(**azeotropic**; vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene** using)
IT Regiochemistry
(in the vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT Thermal decomposition
(of ammonium dichromate into chromium oxide for use as a regioselective hydrofluorination catalyst in a process for the vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)
IT Process control
(of the reactor temp. during the regioselective process for the prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene** using the product as a diluent)
IT Hydrofluorination
(regioselective; vapor-phase prodn. of **1,1,1,2,3,3,3-**

heptafluoropropane from **hydrogen fluoride** and **hexafluoropropylene**)

IT Hydrofluorination catalysts
(regioselective; vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene** using chromium oxide as)

IT **Distillation** columns
(vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene** using)

IT 11118-57-3P, Chromium oxide
RL: CAT (Catalyst use); EPR (Engineering process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PREP (Preparation); PROC (Process); USES (Uses)
(regioselective hydrofluorination catalyst in the vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT 7789-09-5, Ammonium dichromate
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); RGT (Reagent); PROC (Process); RACT (Reactant or reagent)
(thermal decompn. of ammonium dichromate into chromium oxide for use as a regioselective hydrofluorination catalyst in a process for the vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT **7664-39-3, Hydrogen fluoride,** reactions
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); RGT (Reagent); PROC (Process); **RACT (Reactant or reagent)**
(vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PREP (Preparation)
(vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

IT **116-15-4, Hexafluoropropylene**

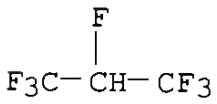
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(vapor-phase prodn. of **1,1,1,2,3,3,3-heptafluoropropane** from **hydrogen fluoride** and **hexafluoropropylene**)

L22 ANSWER 5 OF 24 HCA COPYRIGHT 2004 ACS on STN
137:95519 Hydrofluorination method and catalyst for the manufacture of 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropylene. Golubev, A. N.; Zhukova, V. A.; Novikova, M. D.; Shabalin, D. A.; Zakharov, V. Yu.; Nasonov, Yu. B.; Leyferov, S. E.; Antipenok, V. F.; Zagoskin, N. D.; Dedov, A. S.; Maslyakov, A. I. (OAO "Kirovo-Chepetskii Khimicheskii Kombinat im. B. P. Konstantinova", Russia). Russ. RU 2165918 C2 20010427, No pp. given (Russian). CODEN: RUXXE7. APPLICATION: RU 1998-121879 19981203.

AB 1,1,1,2,3,3,3-Heptafluoropropane is prepd. by the hydrofluorination of hexafluoropropylene with hydrogen fluoride at elevated temp. in the presence of a catalyst and with product isolation by known methods. The hydrofluorination is carried out under adiabatic conditions and activated carbon with an ash content of 10%, not less, is used as the catalyst.

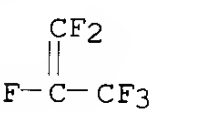
IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(hydrofluorination method and catalyst for the manuf. of 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropylene)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**, Hexafluoropropylene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(hydrofluorination method and catalyst for the manuf. of 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropylene)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



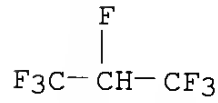
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

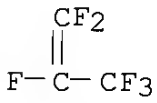
IC ICM C07C019-08
ICS C07C017-087
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67
IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(hydrofluorination method and catalyst for the manuf. of 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropylene)
IT **116-15-4**, Hexafluoropropylene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(hydrofluorination method and catalyst for the manuf. of 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropylene)

L22 ANSWER 6 OF 24 HCA COPYRIGHT 2004 ACS on STN
136:218629 Hydrofluorination and fluorination process for the production of octafluoropropane from **hexafluoropropene**. Ohno, Hiromoto; Ohi, Toshio (Showa Denko K. K., Japan). PCT Int. Appl. WO 2002018305 A2 20020307, 29 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-JP7313 20010827. PRIORITY: JP 2000-260205 20000830; US 2000-PV241838 20001020.
AB Octafluoropropane is produced in high yield and selectivity by: (1) hydrofluorinating **hexafluoropropene** with **hydrogen fluoride** in the gas phase at 150-450° in the presence of a fluorination catalyst to obtain **2H-heptafluoropropane**; and (2) fluorinating the **2H-heptafluoropropane** obtained in step (1) with fluorine gas in the gas phase at 250-500° in the absence of a catalyst to obtain octafluoropropane.
IT **431-89-0P, 2H-Heptafluoropropane**
RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PYP (Physical process); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene**)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4, Hexafluoropropene**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene**)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride**, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene**)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM C07C019-08
ICS C07C017-087; C07C017-10; C07C017-383; H01L021-30
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48
ST octafluoropropane manuf **hexafluoropropene** hydrofluorination fluorination
IT Hydrofluorination catalysts
(chromium oxide with indium and/or zinc and/or nickel for the hydrofluorination **hexafluoropropene** with **HF** into **2H-heptafluoropropane**)
IT Fluorination
Hydrofluorination
(hydrofluorination and fluorination process for the prodn. of

octafluoropropane from **hexafluoropropene**)

IT **Distillation**
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene** using)

IT 7782-41-4, Fluorine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination process for the prodn. of octafluoropropane from **2H-heptafluoropropane** and)

IT 76-19-7P, Octafluoropropane
RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PYP (Physical process); PREP (Preparation); PROC (Process)
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene**)

IT **431-89-0P, 2H-Heptafluoropropane**
RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PYP (Physical process); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene**)

IT **116-15-4, Hexafluoropropene**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene**)

IT **7664-39-3, Hydrogen fluoride**, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene**)

IT 75-43-4, Dichlorofluoromethane
RL: NUU (Other use, unclassified); USES (Uses)
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene** contg.)

IT 75-45-6, Chlorodifluoromethane 75-46-7, Trifluoromethane 75-72-9, Chlorotrifluoromethane 75-73-0, Tetrafluoromethane 76-15-3 76-16-4, Hexafluoroethane 79-38-9, Chlorotrifluoroethylene 354-33-6, Pentafluoroethane 63938-10-3, Chlorotetrafluoroethane
RL: NUU (Other use, unclassified); REM (Removal or disposal); PROC (Process); USES (Uses)
(hydrofluorination and fluorination process for the prodn. of octafluoropropane from **hexafluoropropene** contg.)

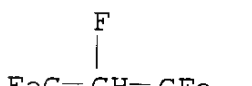
IT 11118-57-3, Chromium oxide
RL: CAT (Catalyst use); USES (Uses)
(hydrofluorination catalyst for the prodn. of **2H-heptafluoropropane** from **hexafluoropropene** and **HF**)

IT 7440-02-0, Nickel, uses 7440-66-6, Zinc, uses 7440-74-6, Indium, uses
RL: CAT (Catalyst use); USES (Uses)
(hydrofluorination catalyst with chromium oxide for the prodn. of **2H-heptafluoropropane** from **hexafluoropropene** and **HF**)

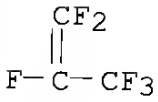
L22 ANSWER 7 OF 24 HCA COPYRIGHT 2004 ACS on STN
135:182382 1,1,1,2,3,3,3-Heptafluoropropane manufacturing process. Nappa, Mario Joseph; Rao, V. N. Mallikarjuna; Sievert, Allen Capron (E. I. Du Pont de Nemours & Co., USA). U.S. US 6281395 B1 20010828, 5 pp. (English). CODEN: USXXAM. APPLICATION: US 1999-283451 19990401. PRIORITY: US 1998-PV80706 19980403.

AB A process is disclosed for the manuf. of CF3CHFCF3 contg. <0.01 ppm (CF3)2C:CF2. The process involves: (a) contacting hexafluoropropene in the vapor phase at <260° with hydrogen fluoride in the presence of a selected fluorination catalyst or produce a product contg. <10 parts (CF3)2C:CF2 per million parts of CF3CHFCF3; and (b) treating the product of (a) as necessary to remove excess (CF3)2C:CF2. Suitable catalysts include: (i) an activated carbon treated to contain from about 0.1-10% of added alkali or alk. earth metals; (ii) three dimensional matrix porous carbonaceous materials; (iii) supported metal catalysts comprising trivalent chromium; and (iv) unsupported chrome oxide prepd. by the pyrolysis of (NH4)2Cr2O7.

IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PUR (Purification or recovery); PREP (Preparation)
(1,1,1,2,3,3,3-heptafluoropropane manufg. process)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4P**, Hexafluoropropene
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); **RACT (Reactant or reagent)**
(1,1,1,2,3,3,3-heptafluoropropane manufg. process using)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(1,1,1,2,3,3,3-heptafluoropropane manufg. process using)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

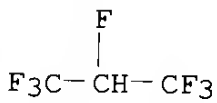
IC ICM C07C017-08
NCL 570165000
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67
IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PUR (Purification or recovery); PREP (Preparation)
(1,1,1,2,3,3,3-heptafluoropropane manufg. process)
IT **116-15-4P**, Hexafluoropropene
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); **RACT (Reactant or reagent)**
(1,1,1,2,3,3,3-heptafluoropropane manufg. process using)
IT **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(1,1,1,2,3,3,3-heptafluoropropane manufg. process using)

L22 ANSWER 8 OF 24 HCA COPYRIGHT 2004 ACS on STN
133:362545 Production of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**. Gibson, Robin Riyadh; Summers, Greg Lyndon (Imperial Chemical Industries PLC, UK). PCT Int. Appl. WO 2000069797 A1 20001123, 18 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-GB1861 20000515. PRIORITY: GB 1999-11475 19990518; US 1999-PV134657 19990518.
AB **1,1,1,2,3,**

3,3-Heptafluoropropane (**HFC 227ea**) is prepd. in high yield and selectivity by reacting **hexafluoropropene** (**HFP**) with **hydrogen fluoride** in a process comprising: (A) charging the reaction mixt. from the reaction of **HFP** with **hydrogen fluoride** to a liq.-phase separator and allowing an org. phase and a **hydrogen fluoride**-rich phase to sep. under gravity; (B) recycling the **hydrogen fluoride** -rich phase sepd. in step (A) to the reactor in which the reaction is carried out; (C) charging the org.-rich phase sepd. in step A to a **distn.** column; (D) recovering the **HFC 227ea** and a **hydrogen fluoride**-rich mixt. sep. from the **distn.** column in step (C); and (E) recycling the **hydrogen fluoride**-rich mixt. recovered from step (D) to the hydrofluorination reactor. Process flow diagrams are presented.

IT **431-89-0P, 1,1,1,2, 3,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(prodn. of **1,1,1,2, 3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride,** reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(prodn. of **1,1,1,2, 3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**)

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

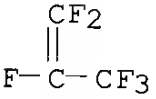
HF

IT **116-15-4, Hexafluoropropene**
RL: RCT (Reactant); **RACT (Reactant or reagent)**

(prodn. of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C017-087
ICS C07C017-38; C07C017-383; C07C019-08

CC 23-3 (Aliphatic Compounds)
Section cross-reference(s): 45, 48, 67

ST heptafluoropropane prepn hydrofluorination **hexafluoropropene**; HFC227EA prepn hydrofluorination **hexafluoropropene**

IT Phase separation
(liq.-liq.; prodn. of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene** and using)

IT **Azeotropes**
(of **1,1,1,2,3,3,3-heptafluoropropane** and **HF** in the prodn. of **1,1,1,2,3,3,3-heptafluoropropane**)

IT Hydrofluorination
(prodn. of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**)

IT **Distillation**
Distillation columns
(prodn. of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene** and using)

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(prodn. of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**)

IT **7664-39-3, Hydrogen fluoride,** reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**

(prodn. of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**)

IT **116-15-4, Hexafluoropropene**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(prodn. of **1,1,1,2,3,3,3-heptafluoropropane** by the hydrofluorination of **hexafluoropropene**)

L22 ANSWER 9 OF 24 HCA COPYRIGHT 2004 ACS on STN
133:351759 Study on preparation of heptafluoropropane in a gas-solid phase catalytic reaction system. Zhong, Guang-Xiang; Chen, Gan-Tang (Zhejiang Chemical Industry Research Institute, Hangzhou, 310023, Peop. Rep. China). Huaxue Fanying Gongcheng Yu Gongyi, 16(3), 251-256 (Chinese) 2000. CODEN: HFGGEU. ISSN: 1001-7631. Publisher: Zhejiangsheng Chuban Duiwai Maoyi Gongsi.

AB 2H-heptafluoropropane (F-227) was prepd. from hexafluoropropene (HFP) and HF by a continuous hydrofluorinating reaction in a gas-solid phase system, and the technol. was systematically studied. When the better catalyst is used, the flux of HFP is 0.33-0.35 kg/h, the mol. ratio of HF to HFP is 1.3-1.5, and the reaction temp. is ≥210°, the F-227 content in the crude gas reaches ≥98.5%.

IT **431-89-0P**, 2H-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(F 227; prepn. of heptafluoropropane in gas-solid phase catalytic reaction system)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

IT **116-15-4**, Hexafluoropropene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(prepn. of heptafluoropropane in gas-solid phase catalytic reaction system)

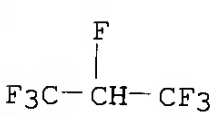
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

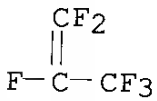
HF

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67
IT **431-89-0P**, 2H-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(F 227; prepn. of heptafluoropropane in gas-solid phase catalytic reaction system)
IT **116-15-4**, Hexafluoropropene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(prepn. of heptafluoropropane in gas-solid phase catalytic reaction system)

L22 ANSWER 10 OF 24 HCA COPYRIGHT 2004 ACS on STN
133:351758 Study on hydrofluorinating catalyst in a gas-solid phase reaction system. Zhong, Guang-Xiang; Chen, Gan-Tang (Zhejiang Chemical Industry Research Institute, Hangzhou, 310023, Peop. Rep. China). Huaxue Fanying Gongcheng Yu Gongyi, 16(3), 245-250 (Chinese) 2000. CODEN: HFGGEU. ISSN: 1001-7631. Publisher: Zhejiangsheng Chuban Duiwai Maoyi Gongsi.
AB A kind of catalysts for prepg. the 2H-heptafluoropropane (F-227) by the hydrofluorination in a gas-solid phase reaction system was studied in detail. The catalyst was prepd. after the active component was infused in carrier, and then the infused carrier was treated by a serial steps of processes. If the quantity of the active component A was 8.5-10% (wt./wt.) on the carrier, the component C2 was 1.0-2.5%, and the total amt. of then was 11%, the catalyst would perform best. When the above catalyst is used for prepg. F-227 from the perfluoropropene and HF, the F-227 content in the crude gas could reach ≥98.5% even at 210°.
IT **431-89-0P**, 2H-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(F 227; hydrofluorinating catalyst in gas-solid phase reaction of perfluoropropene with hydrogen fluoride)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**, Perfluoropropene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(hydrofluorinating catalyst in gas-solid phase reaction of perfluoropropene with hydrogen fluoride)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

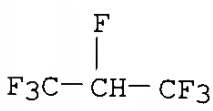
HF

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67
IT **431-89-0P**, 2H-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(F 227; hydrofluorinating catalyst in gas-solid phase reaction of perfluoropropene with hydrogen fluoride)
IT **116-15-4**, Perfluoropropene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(hydrofluorinating catalyst in gas-solid phase reaction of perfluoropropene with hydrogen fluoride)

L22 ANSWER 11 OF 24 HCA COPYRIGHT 2004 ACS on STN
132:153648 Cubic chromium trifluoride and its use for halogenated hydrocarbon processing. Rao, V. N. Mallikarjuna; Subramanian, Munirpallam A. (E. I. Du Pont de Nemours & Co., USA). U.S. US 6028026 A 20000222, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1998-136805 19980820. PRIORITY: US 1997-56792 19970825.
AB This invention provides a cryst. chromium fluoride having a cubic crystal structure (i.e., chromium trifluoride having an X-ray diffraction powder pattern as shown in Table I); and a catalytic compn. comprising cubic chromium trifluoride. This invention also provides a process for changing the fluorine content of halogenated hydrocarbons contg. from one to six carbon atoms, in the presence of a chromium-contg. catalyst. The process is characterized by the chromium-contg. catalyst comprising cubic chromium trifluoride.
IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)

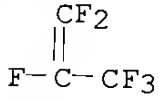
(cubic chromium trifluoride and its use for halogenated hydrocarbon processing)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**, F1216 **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(cubic chromium trifluoride and its use for halogenated hydrocarbon processing)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM B01J027-12
ICS B01J027-132
NCL 502228000
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67
IT 75-10-5P, Difluoromethane 354-33-6P, Pentafluoroethane 374-07-2P, 1,1-Dichloro-1,2,2,2-tetrafluoroethane 420-26-8P, 2-Fluoropropane **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane 593-70-4P, Chlorofluoromethane 811-97-2P, 1,2,2,2-Tetrafluoroethane
RL: IMF (Industrial manufacture); PREP (Preparation)
(cubic chromium trifluoride and its use for halogenated hydrocarbon processing)
IT 75-09-2, Dichloromethane, reactions 115-07-1, Propylene, reactions **116-15-4**, F1216 354-58-5, F113a 359-11-5, F 1123 **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(cubic chromium trifluoride and its use for halogenated

hydrocarbon processing)

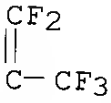
L22 ANSWER 12 OF 24 HCA COPYRIGHT 2004 ACS on STN
131:272325 Processes for the **distillative** purification and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and its **azeotropes** with **HF** in the manufacture of **hexafluoropropene** and **1,1,1,2,3,3-heptafluoropropane**. Miller, Ralph Newton; Rao, V. N. Mallikarjuna; Swearingen, Steven H. (E. I. Du Pont de Nemours & Co., USA). PCT Int. Appl. WO 9951555 A1 19991014, 18 pp. DESIGNATED STATES: W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US7225 19990401. PRIORITY: US 1998-80709 19980403.

AB The sepn. of a mixt. of **HF** and CF3CClFCF3 involves placing the mixt. in a sepn. zone at a temp. of from about -30° to about +100° and at a pressure sufficient to maintain the mixt. in the liq. phase, so that an org.-enriched phase comprising <50 mol percent **HF** is formed as the bottom layer and an **HF**-enriched phase comprising >90 mol percent **HF** is formed as the top layer. The org.-enriched phase is withdrawn from the bottom of the sepn. zone and subjected to **distn.** in a **distn.** column to recover essentially pure CF3CClFCF3. The **distillate** comprising **HF** and CF3CClFCF3 can be removed from the top of the **distn.** column while essentially pure CF3CClFCF3 can be recovered from the bottom of the **distn.** column. The **HF**-enriched phase can be withdrawn from the top of the sepn. zone and subjected to **distn.** in a **distn.** column. The **distillate** comprising **HF** and CF3CClFCF3 can be removed from the top of the **distn.** column while essentially pure **HF** can be recovered from the bottom of the **distn.** column. If desired, the two **distillates** can be recycled back to the sepn. zone. Also disclosed are compns. of **hydrogen fluoride** in combination with an effective amt. of CF3CClFCF3 to form an **azeotrope**-like compn. with **HF**; included are compns. contg. 38.4-47.9 mol percent CF3CClFCF3. Also disclosed are processes for producing **1,1,1,2,3,3,3-heptafluoropropane** and **hexafluoropropene**.

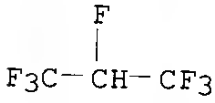
IT **116-15-4P, Hexafluoropropene 431-89-0P, 1,1,1,2,3,3,3**

,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes for the **distillative** purifn. and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and its **azeotropes** with **HF** in the manuf. of **hexafluoropropene** and **1,1,1,2,3,3,3-heptafluoropropane**)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **7664-39-3P, Hydrogen fluoride,** preparation
RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(processes for the **distillative** purifn. and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and its **azeotropes** with **HF** in the manuf. of **hexafluoropropene** and **1,1,1,2,3,3,3-heptafluoropropane**)

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM C07C017-38
ICS C07C017-383; C07C019-10; C07C017-23; C07C019-08; C07C021-18; C07C017-20; C01B007-19
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 23, 48

ST **hexafluoropropene** manuf; heptafluoropropane manuf; **distn** purifn chloroheptafluoropropane

IT Hydrogenolysis
(of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** in the manuf. of **1,1,1,2,3,3,3-heptafluoropropane** and **hexafluoropropene**)

IT Dehydrochlorination
(of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** in the manuf. of **hexafluoropropene**)

IT Fluorination
(of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** with **HF** in the manuf. of **1,1,1,2,3,3,3-heptafluoropropane**)

IT Purification
(processes for the **distillative** purifn. and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and its **azeotropes** with **HF** in the manuf. of **hexafluoropropene** and **1,1,1,2,3,3,3-heptafluoropropane**)

IT **Distillation**
(processes for the **distillative** purifn. and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** with **HF** in the manuf. of **hexafluoropropene** and **1,1,1,2,3,3,3-heptafluoropropane**)

IT **116-15-4P, Hexafluoropropene 431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes for the **distillative** purifn. and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and its **azeotropes** with **HF** in the manuf. of **hexafluoropropene** and **1,1,1,2,3,3,3-heptafluoropropane**)

IT 76-18-6P, Propane, 2-Chloro-1,1,1,2,3,3,3-heptafluoro-
7664-39-3P, Hydrogen fluoride, preparation
RL: PUR (Purification or recovery); RCT (Reactant); PREP

(Preparation); RACT (Reactant or reagent)
(processes for the **distillative** purifn. and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and its **azeotropes** with **HF** in the manuf. of **hexafluoropropene** and **1,1,1,2,3,3,3-heptafluoropropane**)

IT 1652-80-8, 2,2-Dichloro-1,1,1,3,3,3-hexafluoropropane
RL: RCT (Reactant); RACT (Reactant or reagent)
(processes for the **distillative** purifn. and use of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and its **azeotropes** with **HF** in the manuf. of **hexafluoropropene** and **1,1,1,2,3,3,3-heptafluoropropane**)

L22 ANSWER 13 OF 24 HCA COPYRIGHT 2004 ACS on STN
131:258061 Process for the production of **hexafluoropropylene** and **1,1,1,2,3,3,3-heptafluoropropane.** Manogue, William H.; Nappa, Mario Joseph; Sievert, Allen Capron (E. I. Du Pont de Nemours & Co., USA). PCT Int. Appl. WO 9951553 A1 19991014, 16 pp. DESIGNATED STATES: W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US7230 19990401. PRIORITY: US 1998-80708 19980403.

AB **Hexafluoropropylene** and **1,1,1,2,3,3,3-heptafluoropropane** are manufd. by: (A) feeding 1,1,2-trichloro-3,3,3-trifluoro-1-propene, **HF**, and Cl2 to a first reaction zone contg. a trivalent chromium catalyst operated at 250-325° to produce an effluent comprising C3Cl3F5, C3Cl2F6, CF3CClFCF3, HCl, and **HF**; (B) the effluent of step A is **distd.** to produce (i) a low-boiling stream including HCl, (ii) a reactant stream including an **azeotrope** of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** and **HF**, and (iii) a high-boiling stream including C3Cl2F6 and C3Cl3F5; (C) 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** of reactant stream (ii) is reacted with hydrogen in the presence of a catalyst to produce a mixt. of **hexafluoropropylene** and **1,**

1,1,2,3,3,3-heptafluoropropane; (D) the C3Cl2F6 and C3Cl3F5 of high-boiling stream (iii) are fed along with **HF** to a second reaction zone contg. a trivalent chromium catalyst and operated at ≥375° to produce a reaction product comprising CF3CClFCF3 and **HF**; and (E) the product mixt. of step D is recycled to step A. A process flow diagram is presented.

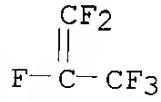
IT **7664-39-3P, Hydrogen fluoride,** preparation
RL: BYP (Byproduct); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3,3-heptafluoropropane**)

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

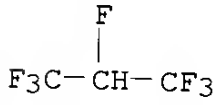
HF

IT **116-15-4P, Hexafluoropropylene 431-89-0P, 1,1,1,2,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PREP (Preparation)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3,3-heptafluoropropane**)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM C07C017-087
ICS C07C017-21; C07C017-23
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 23, 48

ST **hexafluoropropylene** manuf; heptafluoropropane manuf
IT **Distillation**
(in the manuf. of **hexafluoropropylene** and **1,1,2,3,3,3-heptafluoropropane**)
IT Fluorination
(of 1,1,2-trichloro-3,3,3-trifluoro-1-propene with **HF** in the manuf. of **hexafluoropropylene** and **1,1,2,3,3,3-heptafluoropropane**)
IT Hydrogenolysis
(of 2-chloro-**1,1,1,2,3,3,3-heptafluoropropane** in the manuf. of **hexafluoropropylene** and **1,1,2,3,3,3-heptafluoropropane**)
IT **7664-39-3P, Hydrogen fluoride,** preparation
RL: BYP (Byproduct); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3,3-heptafluoropropane**)
IT 1308-38-9, Chromium oxide, uses 7440-15-5, Rhenium, uses 7440-18-8, Ruthenium, uses 10025-73-7, Chromium trichloride
RL: CAT (Catalyst use); USES (Uses)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3,3-heptafluoropropane**)
IT **116-15-4P, Hexafluoropropylene 431-89-0P, 1,1,1,2,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PREP (Preparation)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3,3-heptafluoropropane**)
IT 431-52-7P, 1,1,2-Trichloro-3,3,3-trifluoro-1-propene
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3,3-heptafluoropropane**)
IT 7782-50-5, Chlorine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3,3-heptafluoropropane**)
IT 7647-01-0P, Hydrogen chloride, preparation

RL: BYP (Byproduct); REM (Removal or disposal); PREP (Preparation); PROC (Process)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3, 3,3-heptafluoropropane** using)

IT 7440-47-3D, Chromium, trivalent compds., uses
RL: CAT (Catalyst use); USES (Uses)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3, 3,3-heptafluoropropane** using)

IT 76-18-6P, Propane, 2-Chloro-1,1,1,2,3,3,3-heptafluoro- 28109-69-5P, Trichloropentafluoropropane 42560-98-5P, Dichlorohexafluoropropane
RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3, 3,3-heptafluoropropane** using)

IT 1888-71-7, Perchloropropene
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the prodn. of **hexafluoropropylene** and **1,1,1,2,3, 3,3-heptafluoropropane** using)

L22 ANSWER 14 OF 24 HCA COPYRIGHT 2004 ACS on STN
130:353932 Preparation of fluoroalkanes by the addition reaction of **hydrogen fluoride** with fluoroalkenes and **azeotropic distillation**. Ewing, Paul Nicholas (Imperial Chemical Industries PLC, UK). PCT Int. Appl. WO 9926907 A1 19990603, 22 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-GB3408 19981112. PRIORITY: GB 1997-24831 19971125; US 1997-66836 19971125.

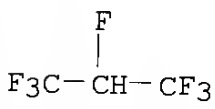
AB **1,1,1,2,3, 3,3-Heptafluoropropane** (I) is prepd. in high yield and selectivity by the addn. reaction of **HF** with **hexafluoropropene**. Both the I and the fluoroalkene sep. form **azeotropes** with **hydrogen fluoride**; the fluoroalkene-**hydrogen fluoride azeotrope** is more volatile than the I-**hydrogen fluoride azeotrope**, which is taken off as a bottoms product. Process flow diagrams are

presented.

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)
(prepn. of fluoroalkanes by the addn. reaction of **hydrogen fluoride** with fluoroalkenes and **azeotropic distn.**)

RN 431-89-0 HCA

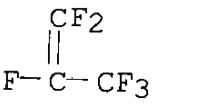
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4, Hexafluoropropene 7664-39-3, Hydrogen fluoride**, reactions
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(prepn. of fluoroalkanes by the addn. reaction of **hydrogen fluoride** with fluoroalkenes and **azeotropic distn.**)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA

CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM C07C017-38
ICS C07C019-08; C07C021-18; C07C017-386; C07C017-087

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48

ST heptafluoropropane manuf **hexafluoropropene** addn reaction **hydrogen fluoride; azeotropic distn** manuf heptafluoropropane

IT **Distillation**
(**azeotropic;** prepn. of fluoroalkanes by the addn. reaction of **hydrogen fluoride** with

fluoroalkenes and **azeotropic distn.**)

IT Hydrocarbons, preparation
RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)
(fluoro, satd.; prepn. of fluoroalkanes by the addn. reaction of **hydrogen fluoride** with fluoroalkenes and **azeotropic distn.**)

IT Alkenes, reactions
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(fluoro; prepn. of fluoroalkanes by the addn. reaction of **hydrogen fluoride** with fluoroalkenes and **azeotropic distn.**)

IT Alkenes, reactions
Alkenes, reactions
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(halo; addn. reaction with **HF** and **azeotropic distn.** with **HF**)

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)
(prepn. of fluoroalkanes by the addn. reaction of **hydrogen fluoride** with fluoroalkenes and **azeotropic distn.**)

IT **116-15-4, Hexafluoropropene 7664-39-3, Hydrogen fluoride**, reactions
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(prepn. of fluoroalkanes by the addn. reaction of **hydrogen fluoride** with fluoroalkenes and **azeotropic distn.**)

L22 ANSWER 15 OF 24 HCA COPYRIGHT 2004 ACS on STN
129:317920 Liquid-phase process and Lewis Acid, transition-metal-fluoride catalysts for the production 1,1,1,2,3,3,3-heptafluoropropane by the hydrofluorination of hexafluoropropene with hydrogen fluoride. Ewing, Paul Nicholas; McCarthy, John Charles (Imperial Chemical Industries PLC, UK). PCT Int. Appl. WO 9850327 A1 19981112, 10 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO

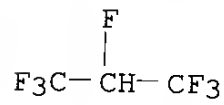
1998-GB1210 19980424. PRIORITY: GB 1997-9268 19970508.

AB 1,1,1,2,3,3,3-Heptafluoropropane is prepd. in high yield and selectivity by the liq.-phase hydrofluorination of hexafluoropropene with HF in the presence of a Lewis acid, transition-metal-fluoride catalyst (e.g., TaF5, NbF5). These catalysts provide an alternative to the use of antimony pentafluoride and, thus, avoid the formation of highly corrosive HSbF6.

IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(liq.-phase process and Lewis Acid transition-metal-fluoride catalysts for the prodn. 1,1,1,2,3,3,3-heptafluoropropane by the hydrofluorination of hexafluoropropene)

RN 431-89-0 HCA

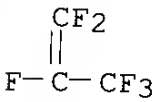
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**, Hexafluoropropene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(liq.-phase process and Lewis Acid transition-metal-fluoride catalysts for the prodn. 1,1,1,2,3,3,3-heptafluoropropane by the hydrofluorination of hexafluoropropene)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA

CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM C07C017-087
ICS C07C019-08; B01J027-12

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67

IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(liq.-phase process and Lewis Acid transition-metal-fluoride

catalysts for the prodn. 1,1,1,2,3,3,3-heptafluoropropane by the hydrofluorination of hexafluoropropene)

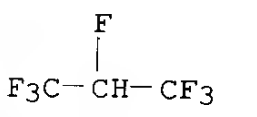
IT **116-15-4**, Hexafluoropropene **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(liq.-phase process and Lewis Acid transition-metal-fluoride catalysts for the prodn. 1,1,1,2,3,3,3-heptafluoropropane by the hydrofluorination of hexafluoropropene)

L22 ANSWER 16 OF 24 HCA COPYRIGHT 2004 ACS on STN
129:246869 Process and antimony pentafluoride catalyst for the addition of hydrofluorocarbons to fluoroolefins. Belen'kii, Gennadii G.; Petrov, Viacheslav A.; Resnick, Paul R. (E. I. Du Pont de Nemours & Co., USA). PCT Int. Appl. WO 9842645 A1 19981001, 12 pp. DESIGNATED STATES: W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US5541 19980319. PRIORITY: RU 1997-106117 19970324.

AB Fluoroalkenes RR1R2CCR1R2F or (FR1R2CCRR2CH2)2 [R = CH3, CH2F, C2H4F, F(CF2)nCH2CH2; n = 1-10; R1 = H, Cl, F, CF3; R2 = H, F, CF3] are prepd. in high yield and selectivity by the addn. reaction of fluorohydrocarbons RF with fluorinated alkenes R1R2C=CR1R2 in the liq. phase in the presence of an antimony pentafluoride catalyst; when (FR1R2CCR1R2CH2)2 is formed, the satd. compd. is CH3CHF2 or CH2FCH2F and anhyd. HF is present. Thus, difluoromethane was added to tetrafluoroethylene in the presence of SbF5 at 50°, producing 1,1,1,2,2,3-hexafluoropropane in 80% yield.

IT **431-89-0P**, Propane, 1,1,1,2,3,3,3-heptafluoro-
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process and antimony pentafluoride catalyst for the addn. of hydrofluorocarbons to fluoroolefins)

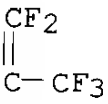
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4 7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process and antimony pentafluoride catalyst for the addn. of

hydrofluorocarbons to fluoroolefins)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM C07C017-26
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67
IT 421-48-7P, 1,1,1,2-Tetrafluoropropane 421-73-8P, Propane, 2-Chloro-1,1,1,2-tetrafluoro- 421-75-0P, 1-Chloro-1,1,2,2-tetrafluoropropane 422-00-4P, Propane, 1,3-Dichloro-1,1,2,2-tetrafluoro- **431-89-0P**, Propane, 1,1,1,2,3,3,3-heptafluoro- 677-56-5P, 1,1,1,2,2,3-Hexafluoropropane 811-97-2P, 1,1,1,2-Tetrafluoroethane 65781-18-2P, Propane, 1,1,1,2,3,3,3-heptafluoro-2-methyl- 65781-19-3P 95576-25-3P, 1,1,1,2,2,5,5,6,6,6-Decafluorohexane 161791-32-8P, Butane, 1,1,1,2,2,3-Hexafluoro- 161791-33-9P, Butane, 1,1,1,2,2,4-Hexafluoro- 213036-32-9P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process and antimony pentafluoride catalyst for the addn. of hydrofluorocarbons to fluoroolefins)
IT 75-37-6, 1,1-Difluoroethane 79-38-9, Chlorotrifluoroethylene 116-14-3, Tetrafluoroethylene, reactions **116-15-4** 359-11-5, Trifluoroethylene 593-53-3, Fluoromethane 598-88-9, 1,2-Dichloro-1,2-difluoroethylene 624-72-6, 1,2-Difluoroethane 1814-88-6, 1,1,1,2,2-Pentafluoropropane **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process and antimony pentafluoride catalyst for the addn. of hydrofluorocarbons to fluoroolefins)

L22 ANSWER 17 OF 24 HCA COPYRIGHT 2004 ACS on STN
126:263838 Continuous process for preparing 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropene and hydrogen fluoride in the presence of hydrogen fluoride-amine salts. Hopp, Peter; Kaufmann, Wolf-Dietmar (Solvay et Cie., Belg.; Hopp, Peter; Kaufmann, Wolf-Dietmar). PCT Int. Appl. WO 9711042 A1 19970327, 10

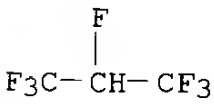
pp. DESIGNATED STATES: W: AL, AU, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (French). CODEN: PIXXD2. APPLICATION: WO 1996-EP4095 19960917. PRIORITY: DE 1995-19534917 19950920.

AB 1,1,1,2,3,3,3-Heptafluoropropane (I) is continuously prepd. by converting hexafluoropropene with HF in the presence of a liq. hydrofluoride salt of an org. base B.(HF)n (B = nitrogenous org. base; n = ≤4) [e.g., Et3N.(HF)2.8], where HF, hexafluoropropene, and the hydrofluoride salt are converted in a first area at a high pressure pl, and after the resulting I is evapd. and isolated from the liq. reaction medium in a second area (at pressure p2 < p1), the remaining liq. reaction medium is recirculated to the first reaction area. A process flow diagram is presented.

IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(continuous process for prepg. 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropene and hydrogen fluoride in the presence of a hydrogen fluoride-amine salt)

RN 431-89-0 HCA

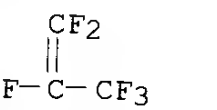
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**, Hexafluoropropene **7664-39-3**, Hydrogen fluoride, reactions **7664-39-3D**, Hydrogen fluoride, amine salts
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(continuous process for prepg. 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropene and hydrogen fluoride in the presence of a hydrogen fluoride-amine salt)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA

CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

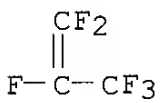
IC ICM C07C017-087
ICS C07C019-08
CC 23-3 (Aliphatic Compounds)
Section cross-reference(s): 45, 48
IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: IMF (Industrial manufacture); PREP (Preparation)
(continuous process for prepg. 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropene and hydrogen fluoride in the presence of a hydrogen fluoride-amine salt)
IT 75-50-3D, Trimethylamine, hydrofluoride salts 102-82-9D, Tributylamine, hydrofluoride salts **116-15-4**, Hexafluoropropene 121-44-8D, Triethylamine, hydrofluoride salts **7664-39-3**, Hydrogen fluoride, reactions **7664-39-3D**, Hydrogen fluoride, amine salts
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(continuous process for prepg. 1,1,1,2,3,3,3-heptafluoropropane from hexafluoropropene and hydrogen fluoride in the presence of a hydrogen fluoride-amine salt)

L22 ANSWER 18 OF 24 HCA COPYRIGHT 2004 ACS on STN
124:342636 Production of 1,1,1,2,3,3,3-heptafluoropropane free of olefin byproducts. Aoyama, Hirokazu; Shibata, Noriaki (Daikin Industries Ltd., Japan). PCT Int. Appl. WO 9602483 A1 19960201, 13 pp. DESIGNATED STATES: W: AU, CA, CN, KR, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1995-JP1379 19950711. PRIORITY: JP 1994-185369 19940714.
AB The 1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) is produced by reacting hexafluoropropene with anhyd. HF in the presence of a Sb catalyst (SbF3, SbF5) under mild conditions (<100°). High conversions up to 99.8% with selectivity >99.9% are obtained with no olefin byproducts. Thus, 15.0g SbF5 was placed in a SUS autoclave and cooled to -30°, followed by adding 40 g anhyd. HF and 50 g hexafluoropropene. The resulting mixt. was stirred at 50° for 4h to give title compd. with 99.8% conversion of reactant and ≥99.9% selectivity.
IT **7664-39-3**, Hydrofluoric acid, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**

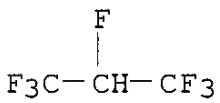
(anhyd.; prodn. of 1,1,1,2,3,3,3-heptafluoropropane free of olefin byproducts)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **116-15-4**, Propene, hexafluoro-
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(prodn. of 1,1,1,2,3,3,3-heptafluoropropane free of olefin byproducts)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: SPN (Synthetic preparation); PREP (Preparation)
(prodn. of 1,1,1,2,3,3,3-heptafluoropropane free of olefin byproducts)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM C07C019-08
ICS C07C017-087; B01J027-12
ICI B01J103-44, B01J105-86
CC 23-3 (Aliphatic Compounds)
Section cross-reference(s): 63
IT **7664-39-3**, Hydrofluoric acid, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(anhyd.; prodn. of 1,1,1,2,3,3,3-heptafluoropropane free of olefin byproducts)
IT **116-15-4**, Propene, hexafluoro-
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(prodn. of 1,1,1,2,3,3,3-heptafluoropropane free of olefin byproducts)
IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: SPN (Synthetic preparation); PREP (Preparation)

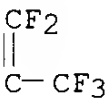
(prodn. of 1,1,1,2,3,3,3-heptafluoropropane free of olefin byproducts)

L22 ANSWER 19 OF 24 HCA COPYRIGHT 2004 ACS on STN
121:82498 Preparing process for hydrofluoric halocarbon and hydrofluoric hydrocarbon. Hu, Changming (Shanghai Organic Chemistry Institute, Chinese Academy of Sciences, Peop. Rep. China). Faming Zhuanli Shenqing Gongkai Shuomingshu CN 1080630 A 19940112, 8 pp. (Chinese). CODEN: CNXXEV. APPLICATION: CN 1992-108469 19920619.

AB CmWgClxBryIz are prepd. via catalytic addn. reaction of CmWnClxBryIz [W = F, H; m = n-6; n+x+y+Z ≤2; m, n, x, y, z = 0-2; m, g ≥2] with HF at 10-200° for 0.5-1 h. Thus, Raney Ni (prepn. given) was used for the addn. reaction of CF2:CF2 with HF at 110° for 4 h to give 100% CF3CHF2 of 99.0% purity.

IT **116-15-4**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(addn. reaction of, with hydrogen fluoride in prepn. of heptafluoropropane)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



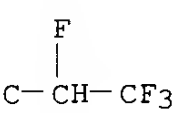
IT **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(addn. reaction of, with tetrafluoroethylene in prepn. of pentafluoroethane)

RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by addn. reaction of hexafluoropropene with hydrogen fluoride)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



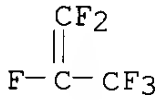
IC ICM C07C019-08
ICS C07C017-00; C07C017-20
CC 23-3 (Aliphatic Compounds)
Section cross-reference(s): 67
IT **116-15-4**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(addn. reaction of, with hydrogen fluoride in prepn. of heptafluoropropane)
IT **7664-39-3**, Hydrogen fluoride, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(addn. reaction of, with tetrafluoroethylene in prepn. of pentafluoroethane)
IT **431-89-0P**, 1,1,1,2,3,3,3-Heptafluoropropane
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by addn. reaction of hexafluoropropene with hydrogen fluoride)

L22 ANSWER 20 OF 24 HCA COPYRIGHT 2004 ACS on STN
118:59239 Reaction of organic compounds with a sulfur tetrafluoride-hydrogen fluoride-halogenating agent system. VII. Reactions of olefins with the SF4-HF-Cl2(Br2) system. Kunshenko, V. B.; Mohamed, Nagib Muhtar; Omarov, V. O.; Muratov, N. N.; Yagupol'skii, L. N. (Odess. Politekh. Inst., Odessa, Ukraine). Zhurnal Organicheskoi Khimii, 28(4), 672-80 (Russian) 1992. CODEN: ZORKAE. ISSN: 0514-7492. OTHER SOURCES: CASREACT 118:59239.
AB Halogenated alkenes undergo halofluorination in SF4-HF-Cl2(Br2) systems. On the basis of Z- and E-1,2-dichloroethenes it was shown that these reactions proceed with anti stereospecificity via bromonium ions. The accumulation of Cl atoms in the alkene mol. hinders electrophilic addn. of stoichiometric equivs. of ClF and BrF to the double bond. The SF4-HF-Br2 system is effective in fluorinating Br-contg. org. compds., wherein only Br atoms on a secondary C are substituted by F.
IT **7664-39-3**, Hydrofluoric acid, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(halofluorination by, with sulfur tetrafluoride and halogen, of olefins)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

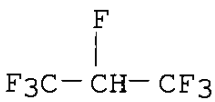
HF

IT **116-15-4**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(halogenation of, by sulfur tetrafluoride-hydrogen fluoride-halogen system)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **431-89-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by halogenation of alkene in sulfur tetrafluoride-hydrogen fluoride-halogen system)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 23-3 (Aliphatic Compounds)
IT **7664-39-3**, Hydrofluoric acid, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(halofluorination by, with sulfur tetrafluoride and halogen, of olefins)
IT 75-01-4, reactions 79-01-6, reactions 79-38-9 106-95-6, reactions 107-05-1 115-07-1, 1-Propene, reactions 116-14-3, reactions **116-15-4** 156-59-2 156-60-5 598-88-9 677-21-4
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(halogenation of, by sulfur tetrafluoride-hydrogen fluoride-halogen system)
IT 76-13-1P 76-14-2P 76-15-3P 76-18-6P 78-75-1P 78-87-5P 79-00-5P 96-11-7P 96-12-8P 96-18-4P 354-14-3P 354-53-0P 354-55-2P 359-28-4P 430-46-6P 430-54-6P 430-57-9P **431-89-0P** 453-01-0P 598-20-9P 816-38-6P 1786-38-5P 1871-72-3P 2106-94-7P 29151-25-5P 32753-89-2P 32753-90-5P 55159-50-7P 55159-51-8P 79719-21-4P 117970-90-8P 145521-33-1P 145521-34-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by halogenation of alkene in sulfur tetrafluoride-hydrogen fluoride-halogen system)

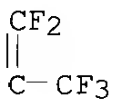
L22 ANSWER 21 OF 24 HCA COPYRIGHT 2004 ACS on STN
59:21317 Original Reference No. 59:3773f-g Octafluoropropane and 2 trifluoromethyl 2 hydrohexafluoropropane. GB 905617 19620912, 3 pp. (Unavailable). PRIORITY: US 19600322.

AB 1,1,1,2,2,3,3,3 Octafluoropropane (I) and F3CCH(CF3)CF3 (II) were prepd. by the process of Brit. 902,590 and by the equipment described therein. During 2.5 hrs., 450 g. 99% heptafluoropropane (III) was passed through the reactor at about 545, the residence time being about 23 sec. Material leaving the reactor was H2O-scrubbed, dried, and condensed in the dry ice trap. A total of 24.6 g **HF** was removed from the exit gas in the H2O and 405.0 g. condensate was collected in the trap. On fractional **distn.**, the following were isolated: 77.0 g. I, b. -38° 6.0 g. hexafluoro-propene (IV),b. -31°; 121 g. III, b. from - 17 to - 18.5° 116 g. II, b. 10-13°; and 81 g. unidentified material, b. .apprx.20°. The present conversion of III to I and II was 16.6 and 26.7, resp. The corresponding yields based on total starting material reacted were 21 and 37%, resp. About 27% by wt. of total recovered products was I and 42% was II. During 1.75 hrs., about 490 g. III was passed through the reactor at about 541°, the residence time being about 15-16 sec. Material leaving the reactor was collected as before. A total of 17.2 g. **HF** was scrubbed from the gas and 464 g. condensate collected. On fractional **distn.** the following were isolated: 35 g. I, 296 g. III, 25 g. II, and 67 g. of higher boiling material. Conversion of III to I and II was 6.6 and 10.7%, resp., and the yields were 16.7 and 27%, resp. Cf. preceding abstr.

IT **116-15-4**, Propene, hexafluoro-
(formation of, in **1,1,1,2,3,3,3-heptafluoropropane** decompn. by heat)

RN 116-15-4 HCA

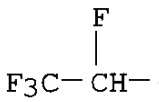
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro-
(pyrolysis(catalytic) of)

RN 431-89-0 HCA

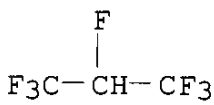
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



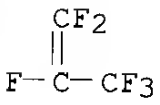
CC 33 (Aliphatic Compounds)

IT Catalysts and Catalysis
(in **1,1,1,2,3,3,3-heptafluoropropane** pyrolysis, active C as)
IT 7440-44-0, Carbon
(catalysts in **1,1,1,2,3,3.3-heptafluoropropane**, pyrolysis)
IT **116-15-4**, Propene, hexafluoro-
(formation of, in **1,1,1,2,3,3,3-heptafluoropropane** decompn. by heat)
IT **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro-
(pyrolysis(catalytic) of)

L22 ANSWER 22 OF 24 HCA COPYRIGHT 2004 ACS on STN
59:21316 Original Reference No. 59:3773d-e Heptafluoropropane. GB 902590 19620801, 3 pp. (Unavailable). PRIORITY: US 19600322.
AB **1,1,1,2,3,3,3 Heptafluoropropane** (I) is made in high yields by hydrofluorination of **hexafluoropropene** (II) in a gas phase process catalyzed by active C. The reactor and catalyst filling were described in U.S. 3,047,640 (CA 58, 448b) for the production of II. During about 125 min., 77 g. anhyd. **HF** and about 308 g. II, premixed, were passed through the reactor at 392-402° with residence time about 9 sec. The effluent gas was scrubbed to remove some **HF**, dried by passage through a CaCl2 tower, and condensed in a dry ice acetone cooled receiver. A total of 36.1 g. **HF** was recovered. **Distn.** of 342 g. condensate gave 316 g. material, b. -16 to -17.5°, and 25 g. still residue all of which (341 g.) was I, 100% yield. During about 120 min., 88 g. **HF** and about 278 g. II, premixed, were passed through the reactor at 300-6° with residence time about 8 sec. A total of 43 g. **HF** was scrubbed out of the reactor exit gas and 316 g. condensate was recovered in the dry ice trap. On **distn.**, 291 g. I and 25 g. I as still residue was obtained, 100% yield.
IT **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro-
(manuf. of)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**, Propene, hexafluoro-
(reaction with **HF**)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrofluoric acid**
(reactions of, with **hexafluoropropene**)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

CC 33 (Aliphatic Compounds)
IT Catalysts and Catalysis
(in **hexafluoropropene** reaction with **HF**,
active C as)
IT 7440-44-0, Carbon
(catalysts in hydrofluorination of **hexafluoropropene**)
IT **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro-
(manuf. of)
IT **116-15-4**, Propene, hexafluoro-
(reaction with **HF**)
IT **7664-39-3, Hydrofluoric acid**
(reactions of, with **hexafluoropropene**)

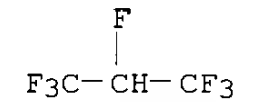
L22 ANSWER 23 OF 24 HCA COPYRIGHT 2004 ACS on STN
58:2973 Original Reference No. 58:448b-d **Hexafluoropropene**.
Sweeney, Richard F.; Woolf, Cyril (Allied Chemical Corp.). US 3047640 19620731, 3 pp. (Unavailable). APPLICATION: US 19600322.
AB Processes were disclosed for the prepn. of **hexafluoropropene** (I) by reaction of 3-chloropentafluoro-1-propene (II) with anhyd. **HF** in the gas phase in the presence of activated C catalyst. During 2.75 hrs. 82 g. **HF** and 429 g. II (premixed) were passed through a Ni tubing packed with activated C with an electric heater enveloping part of the tube. The temp. was held at 194-201° and contact time was about 15 sec. The effluent gas was H2O-scrubbed to remove HCl and **HF**, dried by passage through a CaCl2 tower, and condensed in a dry ice-acetone cooled receiver. On fractional **distn**. of the 421 g. condensate, 135 g. I, b. -29°, 15 g. **1,1,1,2,3,3,3-heptafluoropropane** (III), b. -18.5 to -17°, and 131

g. C2F5Cl, which consisted of about 95% II and about 5% 1-chloropentafluoropropene (IV), b. 8°, and 19 g. 1-chloro-1,1,2,3,3,3-hexafluoropropane (V), b. 16°, were found; about 121 g. material b. 52-3°, corresponding to C3HCl2F5, was also recovered. Conversion of II to I was 49%. During 4 hrs. 170 g. **HF** and 555 g. II were mixed and passed through a reactor contg. 0.47 l. activated C at 204-20° with contact time .apprx.12 sec. On **distn.** of the 500 g. condensate the following were recovered: 132 g. I, 11 g. III, 169 g. C2F5Cl, which consisted of 90% II and about 10% IV, and 52 g. V. About 102 g. material corresponding to C3HCl2F5, b. 52-3°, was also recovered. During 6.5 hrs. a mixt. of 230 g. **HF** and 575 g. II was passed through the reactor at 400-6° with contact time 11 sec. About 355 g. condensate was collected, which on **distn.** gave 27 g. I, 157 g. III, and about 154 g. C2F5Cl consisting of 90% IV and 10% II.

IT **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro-
(prepn. of)

RN 431-89-0 HCA

CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



NCL 260653400

CC 33 (Aliphatic Compounds)

IT 359-58-0, Propane, 1-chloro-1,1,2,3,3,3-hexafluoro- **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro- 13058-05-4, Borazine, 2-chloro-1,3,4,5,6-pentamethyl- 107963-77-9, Dodecane, 1-(acenaphthenyl)-
(prepn. of)

L22 ANSWER 24 OF 24 HCA COPYRIGHT 2004 ACS on STN

55:27441 Original Reference No. 55:5323g-i,5324a-d Substitution and addition reactions of the fluoroolefins. IV. Reactions of fluoride ion with fluoroolefins. Miller, William T., Jr.; Fried, John H.; Goldwhite, Harold (Cornell Univ., Ithaca, NY). Journal of the American Chemical Society, 82, 3091-9 (Unavailable) 1960. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 55:27441.

AB cf. CA 54, 8592b. Fluoride ion reacts readily with fluoroolefins by 3 paths: (1) substitution of vinyl halogen, (2) substitution of allyl halogen with rearrangement, and (3) addn. to form a fluorocarbanion. An example of (1) is the reaction of 1,2-dichlorotetrafluoropropene with KF-HCONH2 to give 55% 2-chloro-1,1,1,3,3,3-hexafluoropropane. Examples of (2) are the

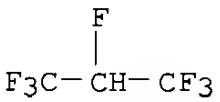
reactions of 3,3-dichloro-1,1,3-trifluoropropene with KF-HCONH2 to give 90% 1-chloro-1,3,3,3-tetrafluoropropene and with Et4NF in CHCl3 to give 74% 1-chloro-1,3,3,3-tetrafluoropropene, 1,3-dichloro-1,2,3,3-tetrafluoropropene with KF-HCONH2 at 60° to give 52% 1,1,1,2,3,3,3-heptafluoropropene, 2,3-dichloro-1,1,3,3-tetrafluoropropene with Et4NF in CHCl3 at 0° to give 52% 2-chloropentafluoropropene in 5 min., and the F ion catalyzed rearrangement of perfluoro-1-heptene to give isomeric olefins. Preferential substitution of allyl, rather than vinyl, halogen is shown by the reaction of 1,4-dibromohexafluoro-2-butene with excess F ion at 60° to give octafluoro-2-butene and its **HF** addn. product. Examples of (3) are the reactions of KF-HCONH2 with chlorotrifluoroethylene to give 72% chlorotetrafluoroethane, with **perfluoropropene** at 25° to give 60% **1,1,1,2,3,3,3-heptafluoropropane**, with **perfluoropropene** at 65° to give 21% **1,1,1,2,3,3,3-heptafluoropropane**, with 2-chloro-1,1,3,3,3-pentafluoropropene at 25° to give 61% 2-chloro-1,1,1,3,3,3-hexafluoropropane, and with perfluoro-2-butene at 81° to give 35% 1,1,1,2,2,3,4,4,4-nonafluorobutane. CCl2FI (209 g.) is charged into a steel lecture cylinder fitted with a steel valve, which is cooled with dry ice, and 60 g. CH2:CF2 condensed into it at 2.5 atm. The cylinder is sealed and heated to 125 ± 5° 19 hrs., then cooled, and vented to yield 12 g. unreacted olefin and by **distn.** CCl2FCH2CF2I (295 g. from 2 runs), b13 39°, n20D 1.4655, d. 2.0978. In the same equipment 316 g. CCl3I and 65 g. CH2:CF2 at 115 ± 5° 36 hrs. give 2 g. olefin and 264 g. CCl3CH2CF2I, b29 83-4°, b22 78.3-8.5°, f.p. -37.5°, n20D 1.5089, d. 2.1157, MRD 43.67, λmax. 270 mμ (ε 379), λmin. 234 mμ (ε 87) (0.67 g./l., iso-octane), coupled by Zn in Et2O to give 88% C6H4Cl6F4, chlorinated to give C6Cl10F4, presumably CCl3CCl2CF2CF2- CCl2CCl3, m. 116.7-18.0°. CCl3CH2CF2I (155 g.) in 400 ml. peroxide-free diethylene glycol di-Et ether is dehydrohalogenated by 57 g. KOH in 70 ml. H2O under N at 150° to give 28.5 g. CCl2:CHCClF2, redistd. through a 100 cm. spinning band column, b749 95.5°, f.p. -96.5°, n20D 1.4290, d. 1.5208, MRD 30.8. Photochem. chlorination at atm. pressure of 16.1 g. CCl2:CHCClF2 gives 16.0 g. CCl3CHCl-CClF2, b746 168-9°, n20D 1.4610, d. 1.725, MRD 40.2. CCl2:-CHCClF2 (2 g.) is chlorinated with 3 g. Cl in the presence of 2.5 g. H2O to give 3.05 g. CCl3CCl2CClF2, m. 51.0-1.2°. Pyrolysis of chlorotrifluoroethylene gives a dichlorotetrafluoropropene fraction, b. 44-9°, which is photochem. brominated, debrominated with Zn in dioxane, treated with LiCl in Me2CO, and then with excess NaI in Me2CO to give CClF:CFCClF2, b733 47.0-8.0°, b. 47.5°, n20D 1.3527, d. 1.5335. CClF2CF:CFCClF2 (1 mole) is

fluorinated by heating with 2 moles HgO and 4.5 moles **HF** at 110° 4 hrs. in a steel bomb to give 73% octafluoro-2-butene.

IT **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro-
(prepn. of)

RN 431-89-0 HCA

CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 10B (Organic Chemistry: Aliphatic Compounds)

IT 360-89-4, 2-Butene, octafluoro- 431-59-4, Propene, 1,3-dichlorotetrafluoro- 431-80-1, Propane, 1,1,1,2,3-pentachloro-3,3-difluoro- 431-87-8, Propane, 2-chloro-1,1,1,3,3,3-hexafluoro- **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro- 460-64-0, Propene, 1,1,3-trichloro-3,3-difluoro- 460-71-9, Propene, 1-chloro-1,3,3,3-tetrafluoro- 460-90-2, Propane, 1,1-dichloro-1,3,3-trifluoro-3-iodo- 661-96-1, Propane, 1,1,1,2,2,3-hexachloro-3,3-difluoro- 680-17-1, Butane, 1,1,1,2,2,3,4,4,4-nonafluoro- 2252-88-2, Propane, 1,1,1-trichloro-3,3-difluoro-3-iodo- 2804-50-4, Propene, 2-chloropentafluoro- 2837-89-0, Ethane, 2-chloro-1,1,1,2-tetrafluoro- 4536-03-2, Hexane, 1,1,1,2,2,5,5,6,6,6-decachloro-3,3,4,4-tetrafluoro-(?)
(prepn. of)

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L23 ANSWER 1 OF 15 HCA COPYRIGHT 2004 ACS on STN

140:201451 Cobalt-substituted chromium oxide compositions, their preparation, and their use as catalysts and catalyst precursors. Nappa, Mario J.; Rao, Velliyur Nott Mallikarjuna; Rosenfeld, David H.; Subramoney, Shekhar; Subramanian, Munirpallam A.; Sievert, Allen C. (E.I. du Pont de Nemours and Company, USA). PCT Int. Appl. WO 2004018093 A2 20040304, 68 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN:

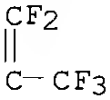
PIXXD2. APPLICATION: WO 2003-US26326 20030821. PRIORITY: US 2002-PV405220 20020822.

AB A cryst. α-chromium oxide where 0.05-6 atom% of the chromium atoms in the α-chromium oxide lattice are replaced by trivalent cobalt (Co+3) atoms is disclosed. Also disclosed is a chromium-contg. catalyst compn. comprising as a chromium-contg. component the cryst. cobalt-substituted α-chromium oxide; and a method for prepg. a compn. comprising the cryst. cobalt-substituted α-chromium oxide. The method involves (a) co-pptg. a solid by adding ammonium hydroxide to an aq. soln. of a sol. cobalt salt and a sol. trivalent chromium salt that contains ≥3 mol of nitrate/mol of chromium in the soln. and has a cobalt concn. 0.05-6 mol% of the total concn. of cobalt and chromium in the soln.; and after at least three moles of ammonium per mol of chromium in the soln. has been added to the soln., (b) collecting the co-pptd. solid formed in (a); (c) drying the collected solid; and (d) calcining the dried solid. Also disclosed is a chromium-contg. catalyst compn. comprising a chromium-contg. component prepd. by treating the cryst. cobalt-substituted -chromium oxide with a fluorinating agent; and a process for changing the fluorine distribution (i.e., content and/or arrangement) in a hydrocarbon or halogenated hydrocarbon in the presence of a catalyst. The process involves using as the catalyst a compn. comprising the cryst. cobalt-substituted α-chromium oxide and/or the treated cobalt-substituted α-chromium oxide.

IT **116-15-4P, Perfluoropropene 431-89-0P, Hfc 227ea**
(cobalt-substituted chromium oxide compns., their prepn., and their use as catalysts and catalyst precursors)

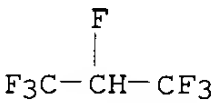
RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 431-89-0 HCA

CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride**, reactions
(cobalt-substituted chromium oxide compns., their prepn., and

their use as catalysts and catalyst precursors)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM B01J023-26
ICS C07C017-20
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
IT 67-66-3P, Hcc 20, preparation 75-01-4P, preparation 75-02-5P 75-35-4P, preparation 75-37-6P 75-43-4P, Hcfc 21 75-45-6P, Hcfc 22 75-46-7P, Hfc 23 75-71-8P, Cfc 12 75-72-9P, Cfc 13 75-88-7P, HCFC 133a 76-11-9P, Cfc 112a 76-13-1P, CFC 113 76-14-2P, Cfc 114 76-15-3P, CFC 115 76-18-6P, CFC 217ba 79-01-6P, preparation 116-14-3P, Perfluoroethylene, preparation **116-15-4P, Perfluoropropene** 354-21-2P, HCFC 122 354-23-4P, HCFC 123a 354-25-6P, HCFC 124a 354-33-6P, HFC 125 354-58-5P, Cfc 113a 359-29-5P 359-35-3P, Hfc 134 374-07-2P, CFC 114a 420-46-2P, Hfc 143a 422-54-8P, Hcfc 224ca 422-57-1P, Hcfc 226ca 431-27-6P 431-53-8P 431-87-8P, Hcfc 226da **431-89-0P, Hfc 227ea** 661-97-2P 690-27-7P, Hfc 1225zc 690-39-1P, Hfc 236fa 812-30-6P 1652-80-8P, CFC 216aa 2252-84-8P, Hfc 227ca 2268-44-2P 2729-28-4P 2804-49-1P
(cobalt-substituted chromium oxide compns., their prepn., and their use as catalysts and catalyst precursors)
IT 74-84-0, Ethane, reactions 74-85-1, Ethylene, reactions 127-18-4, Tetrachloroethylene, reactions 431-52-7 931-91-9, Hexafluorocyclopropane **7664-39-3, Hydrogen fluoride**, reactions 7789-02-8, Chromium trinitrate nonahydrate 16887-00-6, Chloride, reactions 33960-07-5, Cobalt trinitrate hexahydrate
(cobalt-substituted chromium oxide compns., their prepn., and their use as catalysts and catalyst precursors)
IT 74-84-0, Ethane, reactions 74-85-1, Ethylene, reactions 127-18-4, Tetrachloroethylene, reactions 431-52-7 931-91-9, Hexafluorocyclopropane **7664-39-3, Hydrogen fluoride**, reactions 7789-02-8, Chromium trinitrate nonahydrate 16887-00-6, Chloride, reactions 33960-07-5, Cobalt trinitrate hexahydrate
(cobalt-substituted chromium oxide compns., their prepn., and their use as catalysts and catalyst precursors)

L23 ANSWER 2 OF 15 HCA COPYRIGHT 2004 ACS on STN
139:367037 Synthesis and use of hydrofluoroethers, fluoroalkyl ethers, and perfluoroalkyl ethers as novel fire extinguishers. Robin, Mark; Rowland, Thomas F.; Chien, John; Boggs, Janet; Cohn, Mitchel;

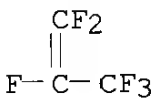
Hedrick, Vicki; Brandstadter, Stephan (USA). U.S. Pat. Appl. Publ. US 2003209685 A1 20031113, 17 pp., Cont.-in-part of Appl. No. PCT/US01/44256. (English). CODEN: USXXCO. APPLICATION: US 2003-435455 20030512. PRIORITY: US 2000-PV249684 20001117; WO 2001-US44256 20011114; US 2002-PV390202 20020620.

AB Highly fluorinated, satd. and unsatd. fluoroethers are used as efficient, economical, and non-ozone-depleting fire extinguishers when used alone or in blends with other fire extinguishers in total flooding and portable fire extinguishing systems. The fluoroalkyl ethers are prepd. by base-catalyzed addn. of a C1-alc. or an alc. to a fluoroalkene, of general structure R1R2C=CXY (R1, R2 = alkyl, fluoroalkyl, or perfluoroalkyl; X, Y are H, I, Br, Cl, or F), to give a fluoroalkyl ether intermediate, of general structure R3-CXY-O-R4 (I; R3 = H, halo, haloalkyl, alkyl, or perfluoroalkyl; X, Y are H, I, Br, Cl, or F; and R4 = alkyl, haloalkyl, or perfluoroalkyl). I can then be fluorinated to yield a desired highly fluorinated fluoroalkyl fluoroalkyl ethers.

IT **116-15-4, Perfluoropropene**
(addn. reaction of, with methanol; synthesis and use of hydrofluoroethers, fluoroalkyl ethers, and perfluoroalkyl ethers as novel fire extinguishers)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride,** reactions
(fluorinating agent; synthesis and use of hydrofluoroethers, fluoroalkyl ethers, and perfluoroalkyl ethers as novel fire extinguishers)

RN 7664-39-3 HCA

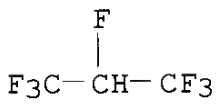
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **431-89-0, 1,1,1,2,3,3,3-Heptafluoropropane**
(secondary fire extinguisher; synthesis and use of hydrofluoroethers, fluoroalkyl ethers, and perfluoroalkyl ethers as novel fire extinguishers)

RN 431-89-0 HCA

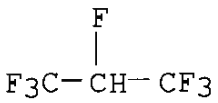
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM A62C002-00
ICS A62D001-00; C07C043-00; C07C041-00
NCL 252002000; 568683000
CC 50-6 (Propellants and Explosives)
Section cross-reference(s): 23
IT 116-14-3, Tetrafluoroethylene, reactions **116-15-4, Perfluoropropene** 690-27-7, 1,1,1,3,3-Pentafluoropropene
(addn. reaction of, with methanol; synthesis and use of hydrofluoroethers, fluoroalkyl ethers, and perfluoroalkyl ethers as novel fire extinguishers)
IT **7664-39-3, Hydrogen fluoride,** reactions
(fluorinating agent; synthesis and use of hydrofluoroethers, fluoroalkyl ethers, and perfluoroalkyl ethers as novel fire extinguishers)
IT 75-46-7, Trifluoromethane 354-33-6, Pentafluoroethane **431-89-0, 1,1,1,2,3,3,3-Heptafluoropropane** 690-39-1, 1,1,1,3,3,3-Hexafluoropropane 2252-84-8, 1,1,2,2,3,3,3-Heptafluoropropane
(secondary fire extinguisher; synthesis and use of hydrofluoroethers, fluoroalkyl ethers, and perfluoroalkyl ethers as novel fire extinguishers)

L23 ANSWER 3 OF 15 HCA COPYRIGHT 2004 ACS on STN
137:249497 Process for producing fluorinated aliphatic compounds by pyrolysis of perfluorocarboxylic acids and their halides and esters. Igumnov, Sergei Mikhailovich; Lekontseva, Galina Ivanovich (Zakrytoe Aktsionernoe Obshchestvo "Altyrskaya Bumazhnaya Fabrika", Russia). Jpn. Kokai Tokkyo Koho JP 2002275106 A2 20020925, 29 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2001-72660 20010314.
AB The pyrolysis is carried out in the presence of a catalyst comprising a carrier most preferably chosen among active carbon, MgO, CaO, BaO, ZnO, Al2O3, NiO, and SiO2 promoted with alkali metal halides selected from the series comprising fluorides, chlorides, bromides, iodides of sodium, potassium, rubidium, cesium at .apprx.100-450° to prep. fluorinated aliph. compds. comprising perfluoroolefins, polyfluoroolefins and their derivs., and optionally, in the presence addnl. of **HF** to form fluorinated aliph. compds. comprising polyfluoroalkanes and their derivs. Thus, pyrolysis of perfluorovaleric acid Me ester using SiO2/KF as catalyst at 240° gave 95.1% perfluoro-2-butene.
IT **431-89-0P**
(catalytic pyrolysis of perfluorocarboxylic acids and their

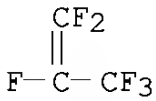
derivs. to fluorinated aliph. compds.)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride**, reactions
(catalytic pyrolysis of perfluorocarboxylic acids and their derivs. to fluorinated aliph. compds.)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **116-15-4P**
(catalytic pyrolysis of perfluorocarboxylic acids and their derivs. to perfluoroolefins)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C017-363
ICS B01J027-12; C07C019-08; C07C021-18; C07C021-185; C07C041-18; C07C043-17; C07B061-00
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 35
IT 354-33-6P **431-89-0P** 680-17-1P 35230-11-6P
(catalytic pyrolysis of perfluorocarboxylic acids and their derivs. to fluorinated aliph. compds.)
IT 356-24-1 376-72-7 378-75-6 422-59-3 422-61-7 426-65-3 663-74-1 677-84-9 **7664-39-3, Hydrogen fluoride**, reactions 87000-86-0 346662-80-4
(catalytic pyrolysis of perfluorocarboxylic acids and their derivs. to fluorinated aliph. compds.)
IT 116-14-3P, preparation **116-15-4P** 357-26-6P 359-11-5P 360-89-4P 1623-05-8P 3823-94-7P 85737-06-0P
(catalytic pyrolysis of perfluorocarboxylic acids and their derivs. to perfluoroolefins)
IT 116-14-3P, preparation **116-15-4P** 357-26-6P 359-11-5P

360-89-4P 1623-05-8P 3823-94-7P 85737-06-0P
(catalytic pyrolysis of perfluorocarboxylic acids and their derivs. to perfluoroolefins)

L23 ANSWER 4 OF 15 HCA COPYRIGHT 2004 ACS on STN
136:325173 Theoretical Study of the Thermal Decomposition Pathways of 2-H Heptafluoropropane. Peterson, Shane D.; Francisco, Joseph S. (Department of Chemistry and Department of Earth and Atmospheric Sciences, Purdue University, West Lafayette, IN, 47907, USA). Journal of Physical Chemistry A, 106(13), 3106-3113 (English) 2002. CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

AB The structures, vibrational frequencies, and energetics of 2-H heptafluoropropane (CF3CHFCF3) as well as the thermal decompn. products and transition-state mols. were studied theor. with both ab initio and d. functional methods. Of a total of 12 primary reaction pathways, two were identified as thermodynamically and kinetically favorable reactions. These are (1) CF3CHFCF3 → CF3CF:CF2 + **HF**, a four-center **HF** elimination pathway, and (2) CF3CHFCF3 → CF3CHF + CF3, a C-C bond fission pathway. The best est. of the ΔHr,298 for these processes are 34.8 and 92.3 kcal/mol using QCISD(T)/6-311G(d,p)//UMP2/6-31G(d) methods, resp. The barrier for CF3CHFCF3 → CF3CF:CF2 + **HF** is 79.5 kcal/mol using the same methods. These results are discussed in light of past and current lab. studies.

IT **431-89-0, 2H-Heptafluoropropane**
(theor. study of thermal decompn. paths of **2H-heptafluoropropane**)

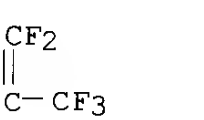
RN 431-89-0 HCA

CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

IT **116-15-4 7664-39-3, Hydrogen fluoride**, properties
(theor. study of thermal decompn. paths of **2H-heptafluoropropane**)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

CC 22-8 (Physical Organic Chemistry)
IT Density functional theory
(B3LYP; theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT MP4 (Moller-Plesset)
(MP4(SDTQ); theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT Bond cleavage
(carbon-carbon; theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT Molecular structure
(optimized; theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT Ab initio methods
Dehydrofluorination
Dehydrofluorination enthalpy
Elimination reaction
Elimination reaction enthalpy
Fragmentation reaction
Fragmentation reaction enthalpy
Molecular vibration
Potential barrier
Potential energy hypersurface
QCISD(T) (molecular orbital)
Reaction enthalpy
Thermal decomposition
Transition state structure
Vibrational frequency
(theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT IR absorption
IR spectra
(theor.; theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT MP2 (Moller-Plesset)
(unrestricted; theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT **431-89-0, 2H-Heptafluoropropane**
(theor. study of thermal decompn. paths of **2H-heptafluoropropane**)
IT 75-46-7, Trifluoromethane 75-73-0, Tetrafluoromethane 76-16-4,

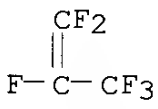
Hexafluoroethane **116-15-4** 354-33-6 359-11-5 431-63-0 690-27-7 811-97-2 2154-59-8, Difluoromethylene 2264-21-3, Trifluoromethyl 3142-79-8 3248-60-0 3369-48-0 **7664-39-3, Hydrogen fluoride,** properties 7782-41-4, Fluorine, properties 13453-52-6 40617-75-2 54041-00-8 58734-91-1 60002-06-4 75995-72-1 414896-87-0 414896-88-1 414896-89-2 414896-90-5 414896-91-6 414896-92-7 414896-93-8 414896-94-9 414896-95-0
(theor. study of thermal decompn. paths of **2H-heptafluoropropane**)

L23 ANSWER 5 OF 15 HCA COPYRIGHT 2004 ACS on STN
134:239309 Fluorinating catalyst for preparing fluoroalkane. Xu, Jinhe; Chen, Zhijun; Yang, Zhenhua; Zhang, Weibiao (Zhejiang Yingguang Chemical Co., Ltd., Peop. Rep. China). Faming Zhuanli Shenqing Gongkai Shuomingshu CN 1263795 A 20000823, 9 pp. (Chinese). CODEN: CNXXEV. APPLICATION: CN 2000-103974 20000318.

AB The catalyst can be formulated by AlF3.aAF3.bBF3.cCF3.dDF2, where A represents trivalent metal element from main group (Sb or Bi), B represents trivalent metal element from subgroup (Cr or Fe), C represents bivalent metal element from main group (Ca, Mg or Ba), and D from bivalent metal element from subgroup (Zn, Co or Ni); a, b, c, d = 0.001-0.01, 0.05-0.15, 0.01-0.05, and 0.01-0.05, resp. The catalyst is prepd. by mixing the raw material, then mixing with 20-40% **HF** soln., filtering, drying, grinding, forming, and activating at 250°. The catalyst can be used to prep. fluoroalkane with carbon no. of 1-3, such as trifluoromethane, difluoromethane, 1,1,1-trifluoro-2-chloroethane, 1,1,1,2-tetrafluoroethane, **1,1,1,2,3,3,3-heptafluoropropane**. The catalyst has high activity, selectivity and stability. A mixed fluoride was used to react **HF** and CHClF2 at 1.5-2 ratio for 15-20 s, giving CHF3 with 99.9% selectivity and 99.6% conversion.

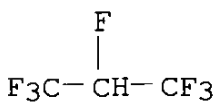
IT **116-15-4P, Hexafluoropropene 431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
(fluorinating catalyst for prepg. fluoroalkane)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX

NAME)



IT **7664-39-3, Hydrogen fluoride,** reactions
(fluorinating catalyst for prepg. fluoroalkane)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

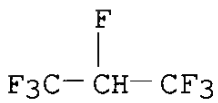
IC ICM B01J027-12
ICS C07C017-00
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67
ST catalyst fluoroalkane fluorinating aluminum fluoride;
hydrogen fluoride fluorination catalyst
trifluoromethane
IT 75-10-5P, Difluoromethane 75-45-6P, Chlorodifluoromethane
75-46-7P, Trifluoromethane 79-01-6P, Trichloroethene, preparation
116-15-4P, Hexafluoropropene 431-89-0P,
1,1,1,2,3,3
,3-Heptafluoropropane 811-97-2P,
1,1,1,2-Tetrafluoroethane 2837-89-0P, R124
(fluorinating catalyst for prepg. fluoroalkane)
IT **7664-39-3, Hydrogen fluoride,** reactions
(fluorinating catalyst for prepg. fluoroalkane)

L23 ANSWER 6 OF 15 HCA COPYRIGHT 2004 ACS on STN
132:51456 Hydrofluorination process and catalysts for the manufacture of **1,1,1,2,3,3**
,3-heptafluoropropane from
perfluoropropene and **hydrogen fluoride.**
Bragante, Letanzio; Cuzzato, Paolo (Ausimont S.p.A., Italy; Solvay Solexis S.p.A.). Eur. Pat. Appl. EP 967192 A1 19991229, 9 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 1999-111562 19990615. PRIORITY: IT 1998-MI1407 19980619.
AB **Perfluoropropene** (I) is subjected to **HF** hydrofluorination in the gas phase to produce **1,1**
,1,2,3,3,3-
heptafluoropropane in high yield nd selectivity using a fluorinated alumina contg. ≥90% AlF3, and, optionally,

trivalent chromium compds., as a catalyst system with a **HF** -I molar ratio of 4-20:1 at 320-420°.

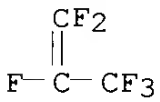
IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
(hydrofluorination process and catalysts for the manuf. of **1,1,1,2,3,3,3-heptafluoropropane** from **perfluoropropene** and **hydrogen fluoride**)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4, Perfluoropropene**
(hydrofluorination process and catalysts for the manuf. of **1,1,1,2,3,3,3-heptafluoropropane** from **perfluoropropene** and **hydrogen fluoride**)

RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C017-08
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67
ST heptafluoropropane manuf **perfluoropropene** hydrofluorination; hydrofluorination catalyst manuf heptafluoropropane
IT Hydrofluorination
Hydrofluorination
(catalysts; fluorinated alumina optionally trivalent chromium compds. for the conversion of **perfluoropropene** and **HF** into **1,1,1,2,3,3,3-heptafluoropropane**)
IT Hydroaddition reaction catalysts
Hydroaddition reaction catalysts
(hydrofluorination catalysts; fluorinated alumina optionally trivalent chromium compds. for the conversion of

perfluoropropene and **HF** into **1,1,1,2,3,3,3-heptafluoropropane**)

IT Hydrofluorination
(of **perfluoropropene** and **HF** in the manuf. of **1,1,1,2,3,3,3-heptafluoropropane**)

IT 1308-38-9, Chromium oxide (Cr2O3), uses 1344-28-1D, Alumina, fluorinated compds. 7440-47-3, Chromium, uses 7784-18-1, Aluminum trifluoride 7784-18-1D, Aluminum fluoride, reaction products with chromium trichloride 7788-96-7, Chromium oxyfluoride 7788-97-8, Chromium(III) fluoride 10025-73-7D, Chromium trichloride, reaction products with aluminum fluoride
(hydrofluorination process and catalysts for the manuf. of **1,1,1,2,3,3,3-heptafluoropropane** from **perfluoropropene** and **hydrogen fluoride**)

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
(hydrofluorination process and catalysts for the manuf. of **1,1,1,2,3,3,3-heptafluoropropane** from **perfluoropropene** and **hydrogen fluoride**)

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
(hydrofluorination process and catalysts for the manuf. of **1,1,1,2,3,3,3-heptafluoropropane** from **perfluoropropene** and **hydrogen fluoride**)

L23 ANSWER 7 OF 15 HCA COPYRIGHT 2004 ACS on STN
130:95231 Shock-Tube Study of the Pyrolysis of the Halon Replacement Molecule CF3CHFCF3. Hynes, Robert G.; Mackie, John C.; Masri, Assaad R. (School of Chemistry, University of Sydney, 2006, Australia). Journal of Physical Chemistry A, 103(1), 54-61 (English) 1999. CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

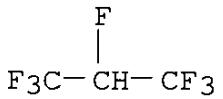
AB The kinetics of pyrolysis of CF3CHFCF3 have been studied in dil. mixts. (0.5 and 3 mol %) in argon in a single-pulse shock tube over the temp. range of 1200-1500 K, residence times behind the reflected shock of between 650 and 850 μs, and pressures between 16 and 18 atm. Fluorinated products were quantified with gas chromatog. and Fourier transform IR spectroscopy; identification of unknown fluorocarbons and hydrofluorocarbons was performed with gas chromatog.-mass spectrometry. The most significant products

detected were C2F6, CF2:CHF, C2F4, C3F6, cyclo-C3F6, and CF3CHFCF2H. Traces of CF3H, CF4, C2F5H, C3F8, C4F6, and isomers of C4F8 were also identified. A detailed kinetic reaction scheme is presented to model the exptl. reactant and product yield profiles as a function of temp. The results of modeling showed that the major initiation reaction was the C-C bond fission reaction. The abstraction of the secondary H atom by F atoms was also predicted to be important, whereas 1,2-**HF** elimination was slower. From expts. and modeling, the following initiation rate consts. were obtained: CF3CHFCF3 → CF3 + CF3CHF (k37 = 1015.9 exp(-355.6 kJ mol-1/RT) s-1), CF3CHFCF3 → C3F6 + **HF** (k38 = 1012.9 exp(-291.2 kJ mol-1/RT) s-1), and CF3CHFCF3 + F → CF3CFCF3 + **HF** (k39 = 1013.6 exp(-10.1 kJ mol-1/RT) cm3 mol-1 s-1).

IT **431-89-0, 1,1,1,2,3,3,3-Heptafluoropropane**
(shock-tube study of pyrolysis of the Halon replacement mol. CF3CHFCF3)

RN 431-89-0 HCA

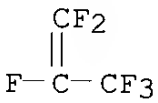
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4P, Hexafluoropropene**
(shock-tube study of pyrolysis of the Halon replacement mol. CF3CHFCF3)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



CC 22-8 (Physical Organic Chemistry)
Section cross-reference(s): 59

IT **431-89-0, 1,1,1,2,3,3,3-Heptafluoropropane**
(shock-tube study of pyrolysis of the Halon replacement mol. CF3CHFCF3)

IT 76-16-4P, Perfluoroethane 116-14-3P, Tetrafluoroethene, preparation **116-15-4P, Hexafluoropropene** 359-11-5P, Trifluoroethene 431-63-0P, 1,1,1,2,3,3-Hexafluoropropane 931-91-9P, Hexafluorocyclopropane
(shock-tube study of pyrolysis of the Halon replacement mol.

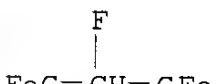
CF3CHFCF3)

L23 ANSWER 8 OF 15 HCA COPYRIGHT 2004 ACS on STN
128:75076 Transformations of F-Alkyl Iodides and Bromides Induced by Nickel(0) Carbonyl. Krespan, Carl G.; Dixon, David A. (DuPont Central Research Development, Experimental Station, Wilmington, DE, 19880-0328, USA). Journal of Organic Chemistry, 63(1), 36-43 (English) 1998. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB Adducts of primary F-alkyl iodides with nickel carbonyl are formed readily in donor solvents and pyrolyze at 100-150° to give olefinic coupling products in high yield. The mechanism proposed to account for the obsd. chem. involves preferential α-elimination of fluorine with formation of a carbenoid species complex coordinated to nickel. Differences in reaction paths among several types of substrate halides are rationalized on the basis of polarization of the Ni-C bond in the adducts. Support for these proposals is provided by state-of-the-art calcns.

IT **431-89-0 7664-39-3, Hydrofluoric acid**, properties
(gas-phase acidity of)

RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

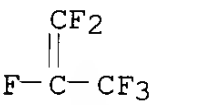


RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **116-15-4**
(heat of formation of)

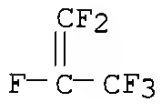
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



CC 22-13 (Physical Organic Chemistry)
Section cross-reference(s): 23, 29

IT 75-46-7 306-83-2 354-33-6 431-71-0 **431-89-0**
433-66-9 2252-84-8 5528-43-8 5595-10-8 **7664-39-3,**
Hydrofluoric acid, properties 16984-48-8,
Fluoride, properties 35476-45-0 35556-60-6 37185-14-1
54128-17-5 127256-66-0 130016-58-9 200502-40-5 200502-43-8
200502-44-9
(gas-phase acidity of)
IT 67-64-1, 2-Propanone, properties 116-14-3, properties
116-15-4
(heat of formation of)

L23 ANSWER 9 OF 15 HCA COPYRIGHT 2004 ACS on STN
128:38788 Experimental study on **2H-heptafluoropropane**
pyrolysis. Ritter, Edward (Department of Chemical Engineering,
Villanova University, Villanova, PA, 19085, USA). Chemical and
Physical Processes in Combustion 209-212 (English) 1997. CODEN:
CPPCD9. ISSN: 0277-1128. Publisher: Combustion Institute.
AB Mixts. of 2% **2H-heptafluoropropane** (CF3CHFCF3)
in N were pyrolyzed at atm. pressure at 1023-1173 K and 0-2 s
reaction time in a quartz tubular flow reactor. Major gas phase
products included: **perfluoropropene,** pentafluoropropene,
perfluorodimethylacetylene, hexafluoroethane, trifluoroethylene,
tetrafluoroethylene, and perfluoroisobutene. **2H-**
heptafluoropropane does not decomp. appreciably at temps.
<1023 K, under study conditions, and requires temps. >1173 K for
complete conversion. The wide assortment of products and rapid
solids formation is consistent with a radical driven chain reaction
and polymn. Dominant reaction pathways involve C-C bond rupture in
addn. to α,β **HF** elimination to
perfluoropropene. At 1173 K, SiF4 was obsd. in the gas
chromatog./mass chromatogram, indicating the onset of attack of the
quartz reactor by **HF.** The absence of SiF4 at temps.
≤1148 K indicates attack on the reactor surface by **HF**
was unimportant under those conditions.
IT **116-15-4, Perfluoropropene 7664-39-3,**
Hydrogen fluoride, processes
(exptl. study of temp. and reaction time effect on reaction
products of **2H-heptafluoropropane**/nitrogen
mixt. pyrolysis at atm. pressure in quartz tubular flow reactor)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



RN 7664-39-3 HCA

CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **431-89-0, 2H-Heptafluoropropane**
(exptl. study of temp. and reaction time effect on reaction products of **2H-heptafluoropropane**/nitrogen mixt. pyrolysis at atm. pressure in quartz tubular flow reactor)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

CC 59-4 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 51, 52
IT Thermal decomposition
(exptl. study of temp. and reaction time effect on reaction products of **2H-heptafluoropropane**/nitrogen mixt. pyrolysis at atm. pressure in quartz tubular flow reactor)
IT 76-16-4, Hexafluoroethane 116-14-3, Tetrafluoroethylene, processes **116-15-4, Perfluoropropene** 359-11-5, Trifluoroethylene 382-21-8, Perfluoroisobutene 692-50-2, Perfluoro2-butyne **7664-39-3, Hydrogen fluoride**, processes 7783-61-1 37145-46-3, Pentafluoropropene
(exptl. study of temp. and reaction time effect on reaction products of **2H-heptafluoropropane**/nitrogen mixt. pyrolysis at atm. pressure in quartz tubular flow reactor)
IT **431-89-0, 2H-Heptafluoropropane**
7727-37-9, Nitrogen, uses
(exptl. study of temp. and reaction time effect on reaction products of **2H-heptafluoropropane**/nitrogen mixt. pyrolysis at atm. pressure in quartz tubular flow reactor)

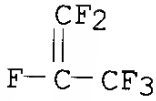
L23 ANSWER 10 OF 15 HCA COPYRIGHT 2004 ACS on STN
127:294947 Regeneration of gas-phase fluorination catalysts. Lacroix, Eric; Cheminal, Bernard; Requieme, Benoit (Elf Atochem S.A., Fr.). Eur. Pat. Appl. EP 798043 A1 19971001, 10 pp. DESIGNATED STATES: R: BE, DE, ES, FR, GB, GR, IT, NL. (French). CODEN: EPXXDW. APPLICATION: EP 1997-400571 19970314. PRIORITY: FR 1996-3972 19960329.
AB Catalysts for gas-phase fluorination are regenerated by treatment of the spent catalyst with Cl and **HF** at 250-450°. A

Cr2O3 catalyst used in converting CF3CH2Cl to CF3CH2F was treated at 350° and atm. pressure for 72 h with a mixt. of 0.25 mol **HF** and 0.01 mol Cl2 per h to restore its activity.

IT **116-15-4, Hexafluoropropene**
(**F 1216**; regeneration of catalysts for fluorination of)

RN 116-15-4 HCA

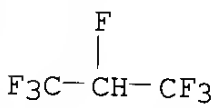
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **431-89-0, 1,1,1,2,3,3,3-Heptafluoropropane**
(**F 227e**; regeneration of fluorination catalysts for manuf. of)

RN 431-89-0 HCA

CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrogen fluoride**, reactions
(in regeneration of fluorination catalysts)

RN 7664-39-3 HCA

CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IC ICM B01J038-42
ICS B01J038-46; B01J027-32

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67

IT **116-15-4, Hexafluoropropene**
(**F 1216**; regeneration of catalysts for fluorination of)

IT **431-89-0, 1,1,1,2,3,3,3-Heptafluoropropane**
(**F 227e**; regeneration of fluorination catalysts for manuf. of)

IT **7664-39-3, Hydrogen fluoride**, reactions
7782-50-5, Chlorine, reactions

(in regeneration of fluorination catalysts)

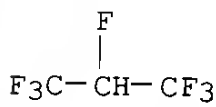
L23 ANSWER 11 OF 15 HCA COPYRIGHT 2004 ACS on STN
124:342630 Reaction of complex amine hydrofluorides with haloalkenes.. Hahn, Ulrich; Franz, Raimund; Siegemung, Guenter (Hoechst A.-G., Germany). Ger. DE 4445529 C1 19960321, 5 pp. (German). CODEN: GWXXAW. APPLICATION: DE 1994-4445529 19941220.

AB R1R2R3N.nHF (R1-R3 = alkyl; R1-R3 together have ≥7 C atoms; 1.5 < n < 3) are reacted with R4CF:CR5R6 (R4 = F, CF3, CF2CF3; R5 = F, Cl, CF3; R6 = H, F, perfluoroalkyl) in such a way that the molar ratio of **HF** to R1R2R3N is reduced enough to allow a separable amine phase to form. Thus, reaction of Bu3N.2.1HF with **hexafluoropropene** at 50° overnight in an autoclave gave 93% F3CCHFCF3 of 95% purity. The liq. residue in the autoclave consisted of a Bu3N phase and a Bu3N.1.9HF phase.

IT **431-89-0P, 1,1,1,2, 3,3,3-Heptafluoropropane**
(reaction of complex amine hydrofluorides with haloalkenes)

RN 431-89-0 HCA

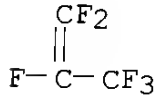
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4, Hexafluoropropene**
(reaction of complex amine hydrofluorides with haloalkenes)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C211-03
ICS C07C211-07; C07C209-82; C07C019-08; C07C017-087

CC 23-3 (Aliphatic Compounds)

IT **431-89-0P, 1,1,1,2, 3,3,3-Heptafluoropropane** 30320-28-6P
(reaction of complex amine hydrofluorides with haloalkenes)

IT **116-15-4, Hexafluoropropene** 1584-03-8, Perfluoro-2-methyl-2-pentene 176720-55-1
(reaction of complex amine hydrofluorides with haloalkenes)

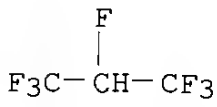
L23 ANSWER 12 OF 15 HCA COPYRIGHT 2004 ACS on STN
122:160066 Process for the addition of **hydrogen fluoride** to haloalkenes. Franz, Raimund; Siegemund, Guenter (Hoechst A.-G., Germany). Eur. Pat. Appl. EP 634383 A1 19950118, 12 pp. DESIGNATED STATES: R: BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, PT, SE. (German). CODEN: EPXXDW. APPLICATION: EP 1994-110535 19940706. PRIORITY: DE 1993-4323264 19930712; DE 1993-4339539 19931119.

AB The title process comprises treating R1CF:R2R3 [R1 = F, CF3, CF2R4; R2 = H, halo, CF3; R3 = H, F, CF3, (halo)alkyl; R4 = (halo)alkyl] with B.nHF (B = N-contg. org. base; n is a whole or fractional no. ≤4).

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
(process for the addn. of **hydrogen fluoride** to haloalkenes)

RN 431-89-0 HCA

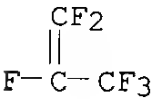
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**
(process for the addn. of **hydrogen fluoride** to haloalkenes)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C017-087
ICS C07C019-08; C07C019-12

CC 23-3 (Aliphatic Compounds)

ST **hydrogen fluoride** addn haloalkene

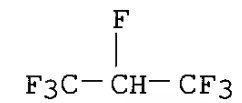
IT 75-88-7P, 1,1,1-Trifluorochloroethane 354-33-6P, Pentafluoroethane **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane** 2837-89-0P, 1,1,1,2-Tetrafluorochloroethane 2924-29-0P, 1,1,1,2,2,4,4,4-Octafluorobutane 30320-28-6P 71127-00-9P, 2-Trifluoromethyl-1,1,1,3,3,4,4,4-Octafluorobutane
(process for the addn. of **hydrogen fluoride** to haloalkenes)

IT 79-38-9 116-14-3, Tetrafluoroethene, reactions **116-15-4**
359-10-4, 1,1-Difluoro-2-chloroethene 359-11-5, Trifluoroethene
760-42-9, 1,1,1,2,4,4,4-Heptafluoro-2-butene 1584-03-8,
Perfluoro-2-methyl-2-pentene 41004-33-5, Perfluoro-2-methyl-2-
butene 161293-36-3 161293-37-4 161293-38-5 161293-39-6
161293-40-9
(process for the addn. of **hydrogen fluoride**
to haloalkenes)

L23 ANSWER 13 OF 15 HCA COPYRIGHT 2004 ACS on STN
122:132563 Preparation of **1,1,1,2**
,3,3,3-heptafluoropropane.
Franz, Raimund; Siegemund, Guenter (Hoechst A.-G., Germany). Eur.
Pat. Appl. EP 634384 A1 19950118, 5 pp. DESIGNATED STATES: R: BE,
CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, PT, SE. (German). CODEN:
EPXXDW. APPLICATION: EP 1994-110536 19940706. PRIORITY: DE
1993-4323054 19930714.

AB The title process comprises treating **hexafluoropropene**
with **HF** in the presence of a tertiary amino group-contg.
ion exchanger.

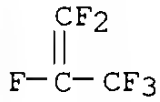
IT **431-89-0P, 1,1,1,2,**
3,3,3-Heptafluoropropane
(prepn. method)
RN 431-89-0 HCA
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX
NAME)



IT **7664-39-3, Hydrofluoric acid**, uses
(prepn. of **1,1,1,2,**
3,3,3-heptafluoropropane)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **116-15-4**
(prepn. of **1,1,1,2,**
3,3,3-heptafluoropropane)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C017-087
ICS C07C019-08
CC 23-3 (Aliphatic Compounds)
ST fluoropropane; **hydrogen fluoride** addn **hexafluoropropene** ion exchanger
IT Ion exchangers
(prepn. of **1,1,1,2,3,3,3-heptafluoropropane**)
IT 9036-92-4, Amberlite IRA 93
(SP; prepn. of **1,1,1,2,3,3,3-heptafluoropropane**)
IT **431-89-0P**, **1,1,1,2,3,3,3-Heptafluoropropane**
(prepn. method)
IT **7664-39-3**, **Hydrofluoric acid**, uses
(prepn. of **1,1,1,2,3,3,3-heptafluoropropane**)
IT **7664-39-3**, **Hydrofluoric acid**, uses
(prepn. of **1,1,1,2,3,3,3-heptafluoropropane**)

L23 ANSWER 14 OF 15 HCA COPYRIGHT 2004 ACS on STN
116:20676 Multistep synthesis of **hexafluoropropylene** from propane and propylene. Webster, James Lang; McCann, Elrey Lorne; Bruhnke, Douglas William; Lerou, Jan Joseph; Manogue, William Henry; Manzer, Leo Ernest; Swearingen, Steven Henry; Trofimenko, Swiatoslaw; Bonifaz, Cristobal (du Pont de Nemours, E. I., and Co., USA). Eur. Pat. Appl. EP 434409 A1 19910626, 33 pp. DESIGNATED STATES: R: DE, FR, GB, IT. (English). CODEN: EPXXDW. APPLICATION: EP 1990-313951 19901219. PRIORITY: US 1989-452402 19891219.

AB **Hexafluoropropylene** (I) is prepd. by (1) chlorofluorination of at least one of propane, propylene, and partially halogenated C3 acyclic hydrocarbons with **HF** and Cl in the presence of a chlorofluorination catalyst to produce CF3CFClCF3 (II) and other chlorofluorocarbons such as C3F4Cl4, C3H5Cl3, CF3CFClCF2Cl, CF3CCl2CF3, and CF3CCl2CCl3 which are mostly recyclable to the same chlorofluorination step to give II and (2) dehalogenation of II to form I in the presence of a CuO-NiO-Cr2O3-CaF2 (and-MoO3) catalyst contg. at least one of K, Cs, or Rb. In this process there is substantially no perfluoroisobutylene produced as a byproduct which is extremely

toxic and is costly to remove and destroy. Thus, Cr2O3.3H2O was charged to an Inconel tubular reactor and treated with a flow of **HF** at 400° for dehydration and thereto **HF** 90, Cl 35, and propylene 1.5 mol/h were fed at 440° and 790 kPa to give II 75, C3F6Cl2 7, C3F5Cl3 5, C3F7H 3, C3F6ClH 5, C3F8 2 and C2F5Cl 2%. A 1:1 (mol) mixt. of H and a II feed contg. II 79, CF3CF2CF2Cl 17, and CF3CCl:CF2 0.7% was passed over a catalyst CuO/NiO/Cr2O3/2.7 CaF2 contg. 7.9 wt.% K at 402° to give 97% I with 63% conversion of II.

IT **7664-39-3, Hydrogen fluoride,** reactions
(chlorofluorination by chlorine and, of propane or propylene, in prepn. of **hexafluoropropylene**)

RN 7664-39-3 HCA

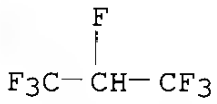
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

IT **431-89-0P, 1,1,1,2,3,3,3-Heptafluoropropane**
(prepn. and conversion of, into **hexafluoropropylene**)

RN 431-89-0 HCA

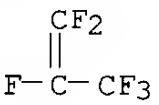
CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4P, Hexafluoropropylene**
(prepn. of, by chlorofluorination and dehalogenation of propane and propylene)

RN 116-15-4 HCA

CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IC ICM C07C019-08
ICS C07C021-18; C07C017-00

CC 23-3 (Aliphatic Compounds)

ST **hexafluoropropylene** prepn chlorofluorination propylene propane; dehalogenation chlorohexafluoropropane catalyst

IT Dehalogenation catalysts
(copper oxide-nickel oxide-chromium oxide-molybdenum oxide contg.

potassium, for chloroheptafluoropropane to **hexafluoropropylene**)

IT Halogenation
(chlorofluorination, of propylene or propane, in prepn. of **hexafluoropropylene**)

IT 1308-38-9, Chromium oxide (Cr2O3), uses 1310-58-3, Potassium hydroxide, uses 1313-27-5, Molybdenum(VI) oxide, uses 1313-99-1, Nickel(II) oxide, uses 1317-38-0, Copper(II) oxide, uses 7440-09-7, Potassium, uses 7440-17-7, Rubidium, uses 7440-46-2, Cesium, uses 7789-75-5, Calcium fluoride, uses 10294-40-3, Barium chromate 11104-65-7, Copper chromite 13548-38-4, Chromium nitrate
(catalyst contg., for dehalogenation of chloroheptafluoropropane to **hexafluoropropylene**)

IT 1307-96-6, Cobalt(II) oxide, uses 1308-14-1, Chromium(III) hydroxide 1308-38-9, Chromium oxide, uses 7440-00-8, Neodymium, uses 7447-39-4, Copper chloride (CuCl2), uses 7447-40-7, Potassium chloride, uses 7646-79-9, Cobalt chloride, uses 7646-85-7, Zinc chloride, uses 7705-08-0, Iron(III) chloride, uses 7784-18-1, Aluminum trifluoride 7788-97-8, Chromium(III) fluoride 7790-86-5, Cerium(III) chloride 10025-73-7, Chromium(III) chloride 10049-07-7, Rhodium(III) chloride 10099-58-8, Lanthanum chloride (LaCl3) 10361-79-2, Praseodymium(III) chloride 10361-82-7, Samarium(III) chloride 10361-92-9, Yttrium chloride (YCl3) 11099-02-8, Nickel oxide 12018-01-8, Chromium oxide (CrO2) 38180-97-1 136254-46-1, Cerium chromium lanthanum oxide (Ce0.2CrLa0.8O3) 137952-95-5 137972-03-3, Chromium zirconium oxide (Cr0.5Zr0.5O1.5-2)
(catalyst, for chlorofluorination of propane or propylene, in prepn. of **hexafluoropropylene**)

IT 7783-70-2, Antimony pentafluoride
(catalyst, for dehalogenation of chloroheptafluoropropane to **hexafluoropropylene**)

IT 74-98-6, Propane, reactions 115-07-1, 1-Propene, reactions
(chlorofluorination and dehalogenation of, **hexafluoropropylene** from)

IT **7664-39-3, Hydrogen fluoride**, reactions
(chlorofluorination by chlorine and, of propane or propylene, in prepn. of **hexafluoropropylene**)

IT 7782-50-5, Chlorine, reactions
(chlorofluorination by **hydrogen fluoride** and, of propane or propylene, in prepn. of **hexafluoropropylene**)

IT 7440-50-8, Copper, reactions 7440-66-6, Zinc, reactions
(dehalogenation by, of chloroheptafluoropropane to **hexafluoropropylene**)

IT 422-86-6P, 1-Chloroheptafluoropropane 431-52-7P, 3,3,3-Trifluoro-1,1,2-trichloropropylene **431-89-0P**,

1,1,1,2,3,3
,3-Heptafluoropropane 661-97-2P,
1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane 1599-41-3P
1652-80-8P, 2,2-Dichloro-1,1,1,3,3,3-hexafluoropropane 1652-89-7P
2252-84-8P, 1,1,2,2,3,3,3-Heptafluoropropane 2268-44-2P,
1,1,2,2-Tetrachloro-1,3,3,3-tetrafluoropropane 2729-28-4P,
1,1-Dichloro-1,2,2,3,3,3-hexafluoropropane 2804-50-4P
28109-69-5P 29470-95-9P 51346-64-6P, 2-Chloro-1,1,2,3,3,3-
hexafluoropropane 75431-43-5P 111548-56-2P 128903-21-9P,
2,2-Dichloro-1,1,3,3,3-pentafluoropropane 136128-45-5P
136150-58-8P
(prepn. and conversion of, into **hexafluoropropylene**)

IT 76-18-6P, 2-Chloro-1,1,1,3,3,3-hexafluoropropane
(prepn. and dehalogenation of, **hexafluoropropylene** from)

IT 76-18-6P, 2-Chloro-1,1,1,3,3,3-hexafluoropropane
(prepn. and dehalogenation of, **hexafluoropropylene** from)

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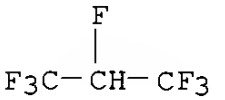
55:48275 Original Reference No. 55:9254g-h Addition of hydrogen halides to fluoroolefins. Knunyants, I. L.; Shokina, V. V.; Kuleshova, N. D. (Inst. Heteroorg. Compds., Moscow). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya 1693-5 (Unavailable) 1960. CODEN: IASKA6. ISSN: 0002-3353.

AB Heating 30 g. CF3CF:CF2 with 100 g. 30% **HF** and 3 g. catalyst (3:1 C-CaSO4 dried at 200°) at 200° in a steel ampul gave after 100 hrs. 80% CF3CHFCF3, b. -17°. Similar reaction with dry HCl run in a flow system over the above catalyst at 230° gave 60% CF3CHFCF2Cl, b. 16°, doo 1.519. Similar reaction with dry HBr gave 50% CF3CHFCF2Br, b. 36°. Similar reactions with (CF3)2C:CF2 at 200° gave: 75% (CF3)2CHCF3, b. 11°; 45% (CF3)2CHCF2Cl, b. 43°, doo 1.591, n20D 1.298; and 50% (CF3)2CHCF2Br, b. 56°, 1.872, 1.318. Also reported was CF3CFBrCF2Br, b. 71°, formed from **perfluoropropylene**. Addn. of HI could not be accomplished under various conditions tried. The products readily lost H halides in the presence of bases.

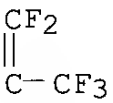
IT **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro-
(prepn. of)

RN 431-89-0 HCA

CN Propane, 1,1,1,2,3,3,3-heptafluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **116-15-4**, Propene, hexafluoro-
(reaction with H halides)
RN 116-15-4 HCA
CN 1-Propene, 1,1,2,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)



IT **7664-39-3, Hydrofluoric acid**
(reactions of, with fluorinated olefins)
RN 7664-39-3 HCA
CN Hydrofluoric acid (8CI, 9CI) (CA INDEX NAME)

HF

CC 10B (Organic Chemistry: Aliphatic Compounds)
IT 359-58-0, Propane, 1-chloro-1,1,2,3,3,3-hexafluoro- 382-24-1, Propane, 1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)- **431-89-0**, Propane, 1,1,1,2,3,3,3-heptafluoro- 661-95-0, Propane, 1,2-dibromohexafluoro- 1559-48-4, Propane, 1-chloro-1,1,3,3,3-pentafluoro-2-(trifluoromethyl)- 1559-50-8, Propane, 1-bromo-1,1,3,3,3-pentafluoro-2-(trifluoromethyl)- 2252-78-0, Propane, 1-bromo-1,1,2,3,3,3-hexafluoro-
(prepn. of)
IT **116-15-4**, Propene, hexafluoro- 382-21-8, Propene, pentafluoro-2-(trifluoromethyl)-
(reaction with H halides)
IT 7647-01-0, Hydrochloric acid **7664-39-3**, **Hydrofluoric acid**
(reactions of, with fluorinated olefins)